Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Environment dependent photophysical and fluorescence turn-off sensing property of Fe(III) by substituted phenyl isochromenopyrrol-5-ones

Roni Boss[††], Milind Shrinivas Dangate [††], R Nishanth Rao[†], Balamurali M M[††]* and Kaushik Chanda[†]*

[††] Chemistry Division, School of Advanced Sciences, Vellore Institute of Technology, Chennai campus, Chennai 600127, Tamilnadu, India

[†] Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, India

E-mail: mmbala@gmail.com

chandakaushik1@gmail.com

Contents

S1: General synthetic procedure for 3-acetyl-2-methyl-1-substitutedphenylisochromeno[4,3-b]pyrrol-5(1*H*)-one (4a-f).[38]

An equimolar mixture of acetylacetone **1** (1.1 mmol), primary amine **2** (1.1 mmol) and MK-10 (10 mg) were taken in a round bottom flask and were heated at 85 ^{o}C for 15 to 30 min, then the reaction mixture was poured into ninhydrin, **3** (1.1 mmol) with occasional shaking and stirred about 90 min at room temperature. The completion of the reaction was monitored by TLC. On completion, the reaction mixture was cooled to room temperature and then quenched by pouring this mixture over crushed ice. The solid formed was allowed to stand for 30 min and filtered off to dryness to obtain the intermediate **3**. To the solution of intermediate **3** in acetic acid (5 mL), 0.5 mL of conc. H_2SO_4 was added and refluxed for 1 hour at 85 ^{o}C. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature and poured over crushed ice with continuous stirring. The solid formed was allowed to stand for 20 min and then filtered. Further purification was done by column chromatography using 10 % EA in Hex as the eluent to afford the substituted isochromenopyrrolones **4** in excellent yields.

3-Acetyl-2-methyl-1-phenylisochromeno[4,3-*b*]pyrrol-5(1*H*)-one (4a)[38]

Pale brown solid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3H), 2.73 (s, 3H), 6.36 (s, 1H), 7.31-7.26 (m, 2H), 7.37 (s, 1H), 7.64-7.60 (m, 4H), 8.34 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.4, 31.6, 118.2, 124.0, 124.4, 125.0, 125.9, 126.9, 127.3, 130.4, 130.7, 131.9, 132.0, 134.9, 135.7, 136.8, 139.0, 139.3, 190.4, 201.3; IR (cm^{-1}, KBr) 3057, 2918, 1712, 1612, 1494; MS (GC-MS) 317; HRMS (EI, m/z); calcd for $C_{20}H_{15}NO_3$: m/z 317.1052; Found 317.1076.

3-acetyl-2-methyl-1-*p*-tolylisochromeno[4,3-b]pyrrol-5(1*H*)-one (4b)[38]

Pale brown solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H), 2.55 (s, 3H), 2.74 (s, 3H), 6.47-6.45 (d, J = 8.2 Hz, 1H), 7.29-7.25 (m, 3H), 7.37 (d, J = 7.6 Hz, 1H), 7.43 (d, J = 7.6 Hz, 2H), 8.33 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.6, 13.7, 20.5, 96.11, 112.5, 117.4, 117.5, 124.5, 126.5, 126.8, 131.2, 131.6, 131.8, 133.3, 134.5, 136.0, 137.4, 139.0, 142.5, 163.2, 190.4; IR (cm^{-1}, KBr) 3199, 2966, 1786, 1670, 1606; MS (GC-MS) 332 (M+H); HRMS (EI, m/z); calcd for $C_{21}H_{17}NO_3$: m/z 331.1208; Found 331.1234.

3-acetyl-1-(2,4-dimethylphenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one (4c):

Pale brown solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 (s, 3H), 2.36 (s, 3H), 2.51 (s, 3H), 2.77 (s, 3H), 6.36 (d, J = 8.0 Hz, 1H), 7.12 (s, 1H), 7.30 (d, J = 7.6 Hz, 1H), 7.39-7.35 (m, 3H), 8.38 (t, J = 1.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.2, 16.7, 20.9, 31.3, 110.3, 111.8, 117.6, 125.6, 128.8, 130.6, 131.2, 131.4, 131.8 (2C), 133.4, 134.9, 135.7, 137.9(2C), 138.9, 140.9, 162.0, 193.7; IR (cm^{-1}, KBr) 3059, 3020, 2920, 1701, 1618, 1467; MS (GC-MS) 346 (M+H); HRMS (EI, m/z); calcd for $C_{22}H_{19}NO_3$: m/z 345.1365; Found 345.1351.

3-acetyl-1-(2, 6-diethylphenyl)-2-methylisochromeno [4, 3-b] pyrrol-5(1*H*)-one (4d)[38]

Pale brown solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01-1.05 (s, 6H), 2.23 (m, 4H), 2.32 (s, 3H), 2.79 (s, 3H), 6.27 (d, J = 5.0 Hz, 1H), 7.28 (d, J = 5.0 Hz, 1H), 7.30 (d, J = 10 Hz, 1H), 7.33-7.37 (m, 2H), 7.55-7.57 (m, 1H), 8.35-8.36 (dd, J = 1.5, 1.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.2, 2×13.7, 2×23.7, 31.3, 110.4, 111.5, 117.7, 117.8, 2×125.6, 2×127.1, 130.5, 130.6, 131.7, 133.8, 134.9, 138.8, 141.0, 142.1, 161.9, 193.6; IR (cm^{-1}, KBr) 3388, 3199, 3057, 2966, 1732, 1668, 1462; MS (GC-MS) 374 (M+H); HRMS (EI, m/z); calcd for $C_{24}H_{23}NO_3$: m/z 373.1678; Found 373.1648.

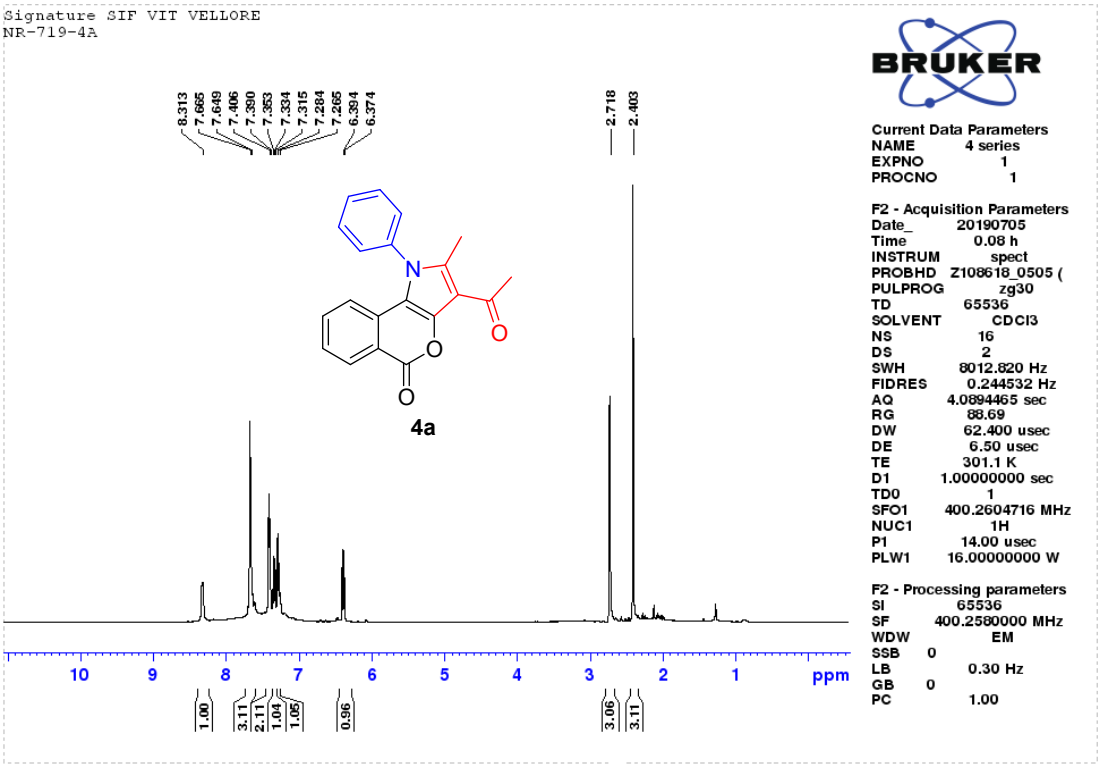
3-acetyl-1-(4-methoxyphenyl)-2-methylisochromeno[4,3-*b*]pyrrol-5(1*H*)-one (4e):

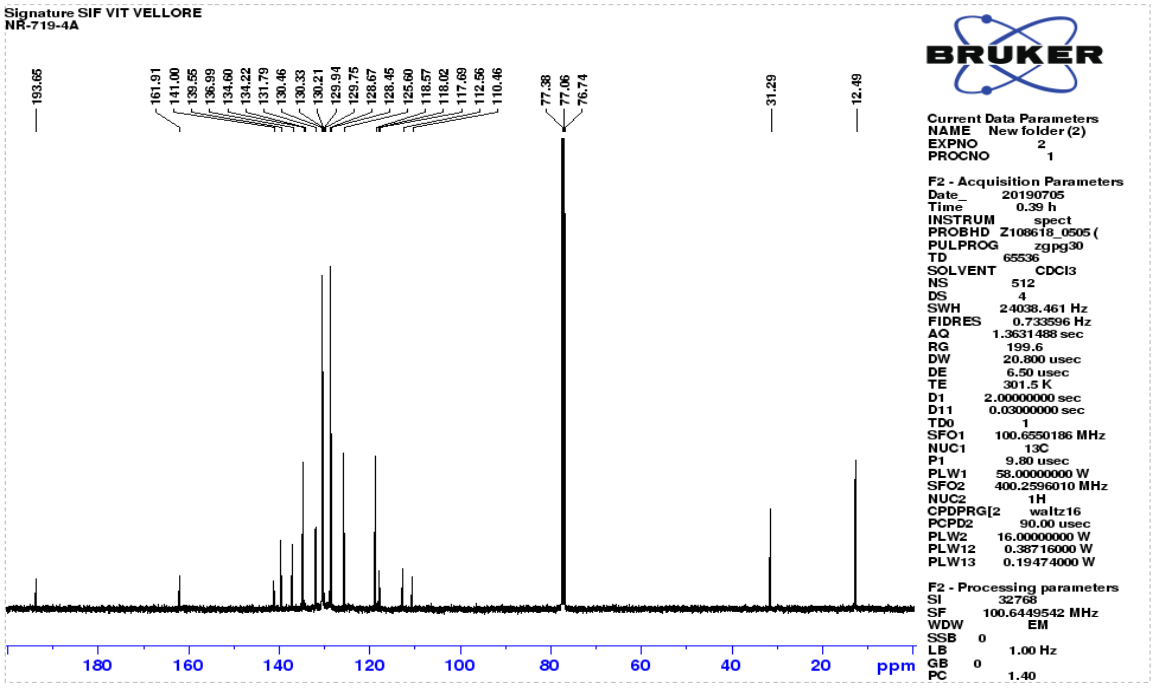
Pale brown solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 2.75 (s, 3H), 3.97 (s, 3H), 6.50 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.7 Hz, 2H), 7.31–7.28 (m, 3H), 7.41-7.37 (m, 1H), 8.35 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.4, 31.3, 55.7, 110.4, 112.7, 115.3, 117.7, 118.6, 124.4, 125.5, 129.4, 130.6, 2×131.8, 134.6, 2×139.9, 140.9, 162.0, 193.6; IR (cm^{-1}, KBr) 2966, 2839, 1716, 1658, 1502; MS (GC-MS) 348 (M+H); HRMS (EI, m/z); calcd for $C_{21}H_{17}NO_4$: m/z 347.1158; Found 347.1108.

3-acetyl-1-(4-chlorophenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one (4f):

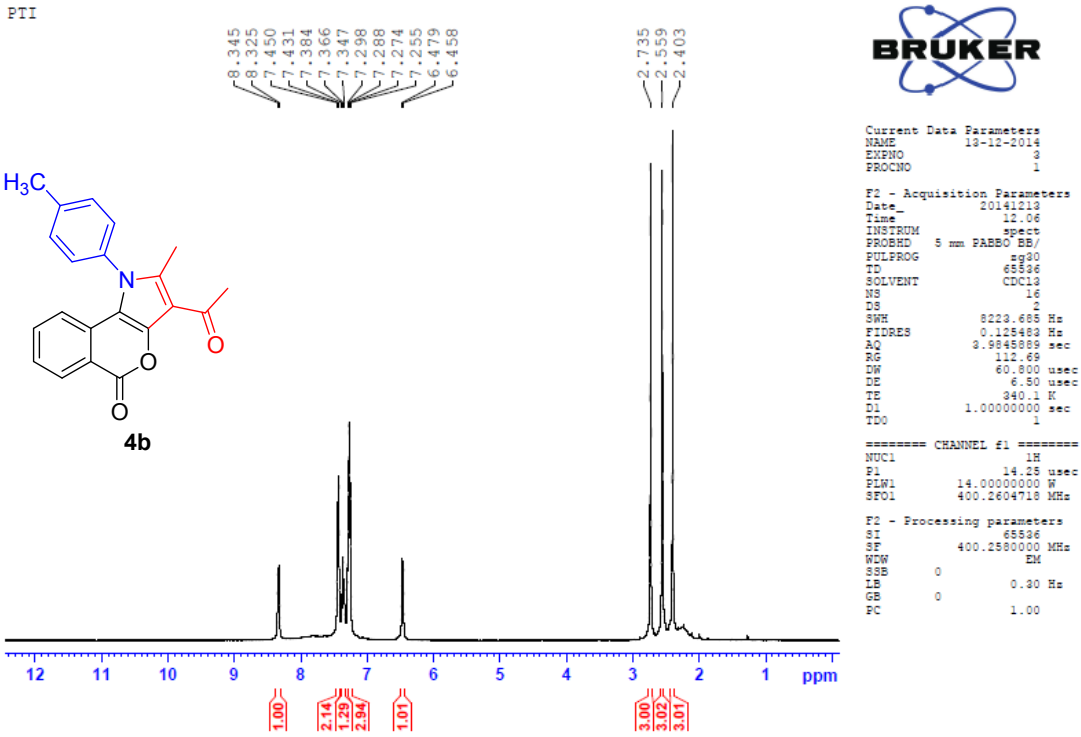
Pale yellow solid, ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.31 (s, 3H), 2.64 (s, 3H), 6.37 (d, J = 8.0 Hz, 1H), 7.19 (s, 1H), 7.24 (d, J = 6.0 Hz, 1H), 7.34-7.28 (m, 2H), 7.55 (d, J = 8.0 Hz, 2H), 8.26 (d, J = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 12.4, 31.3, 110.3, 112.5, 117.7, 118.3, 2×125.8, 129.8, 130.2, 130.6, 132.0, 134.7, 135.5(2C), 136.3, 139.4, 141.1, 161.7, 193.6; IR (cm^{-1}, KBr): 2921, 1712, 1660, 1490, 756; MS (GC-MS) 352 (M+H); HRMS (EI, m/z); calcd for $C_{20}H_{14}ClNO_3$: m/z 351.0662; Found 351.0691.

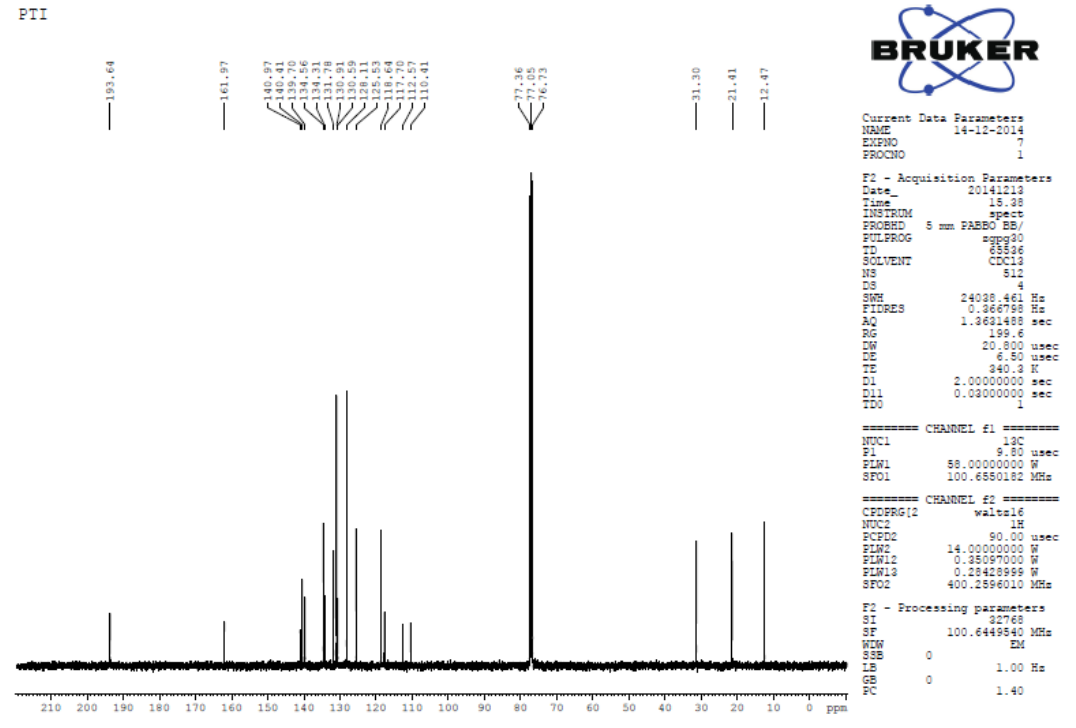
S2: ^{1}H&^{13}C Spectrum of 3-acetyl-2-methyl-1-phenylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4a**



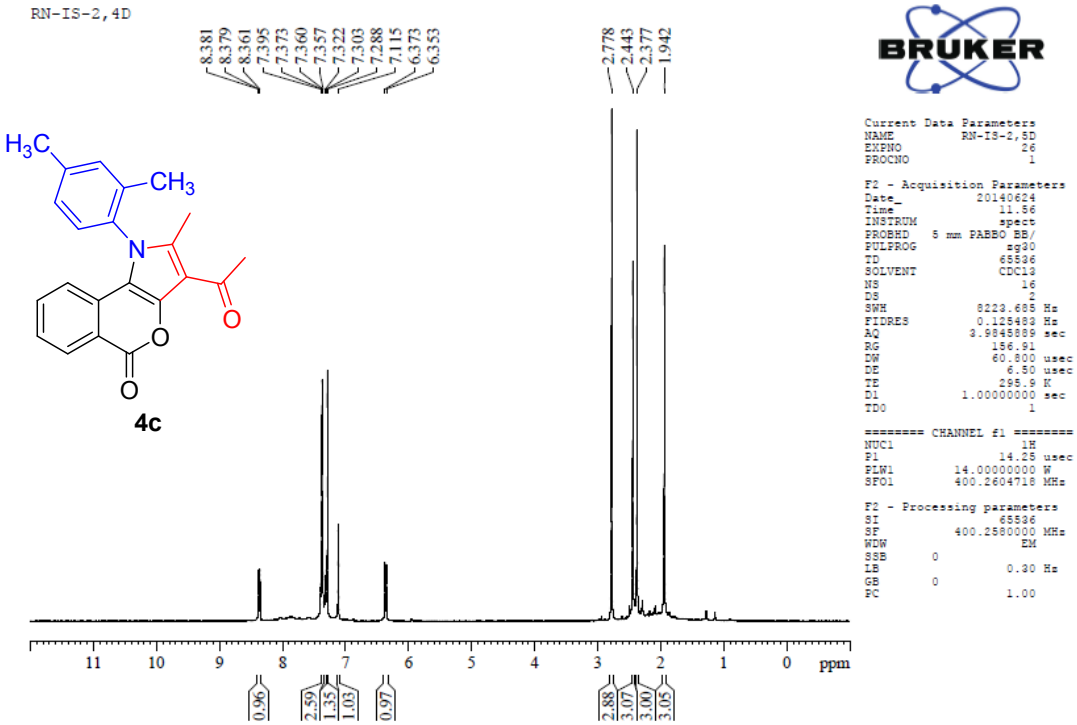


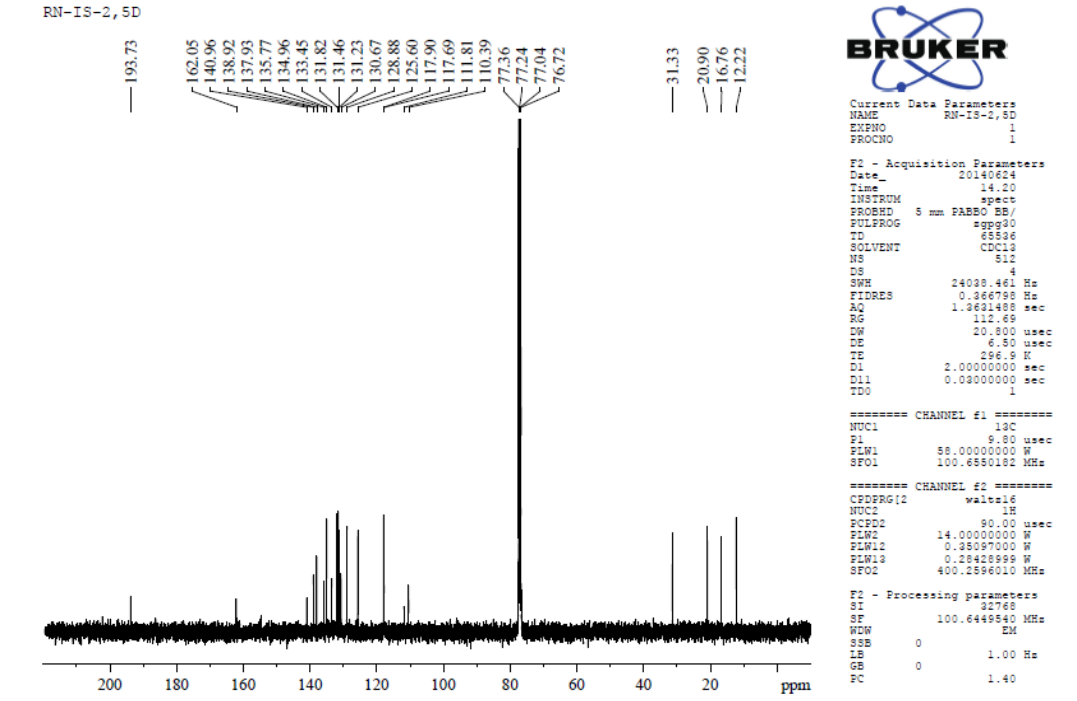
^{1}H &^{13}C NMR Spectrum of 3-acetyl-2-methyl-1-*p*-tolylisochromeno[4,3-*b*]pyrrol-5(1*H*)-one, **4b**



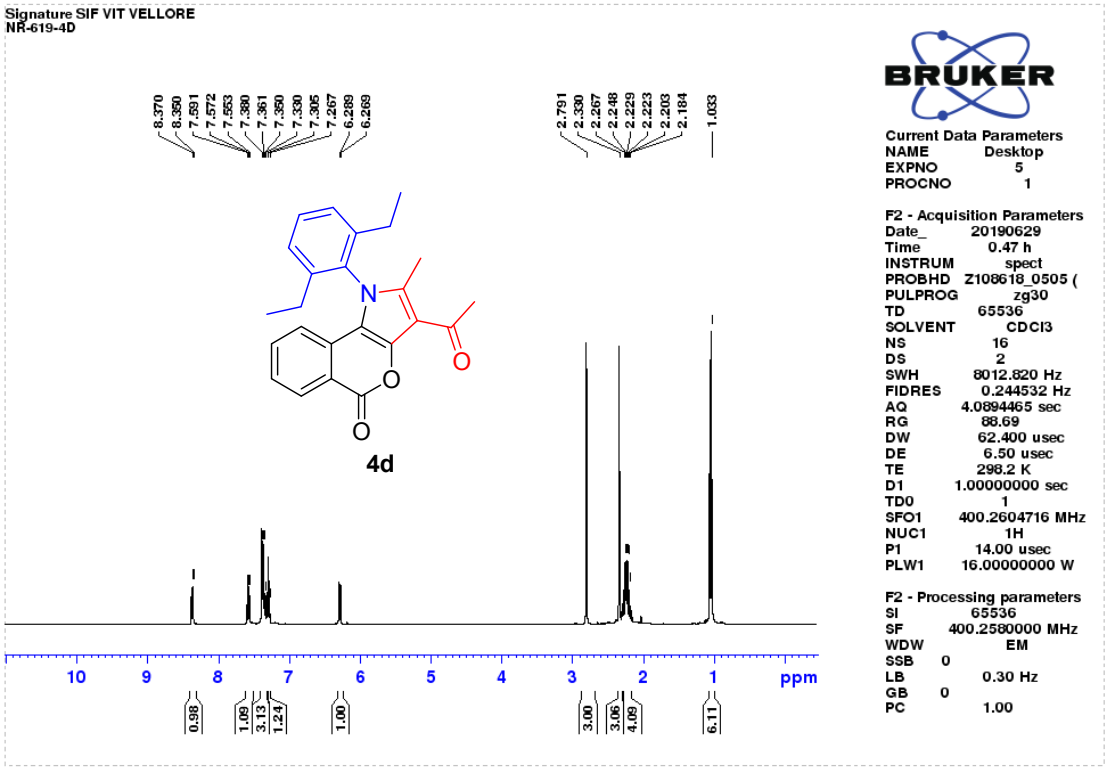


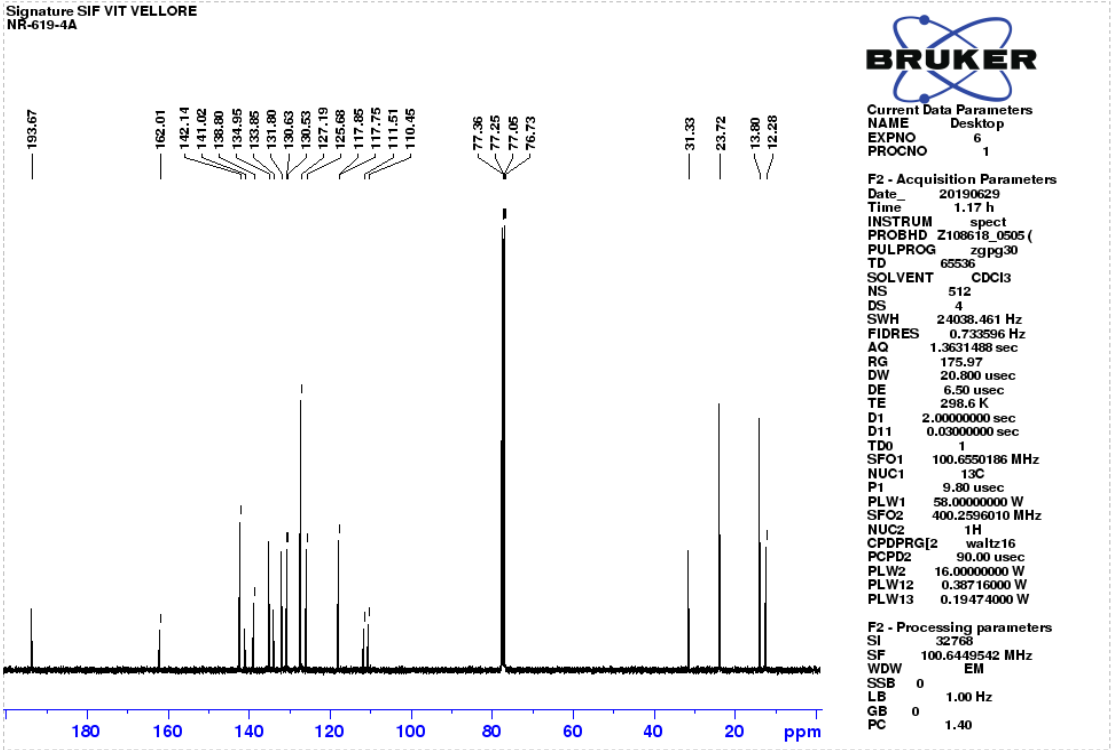
^{1}H &^{13}C NMR Spectrum of 3-acetyl-2-methyl-1-(2,4-dimethylphenyl)isochromeno[4,3-b]pyrrol-5(1*H*)-one, **4c**



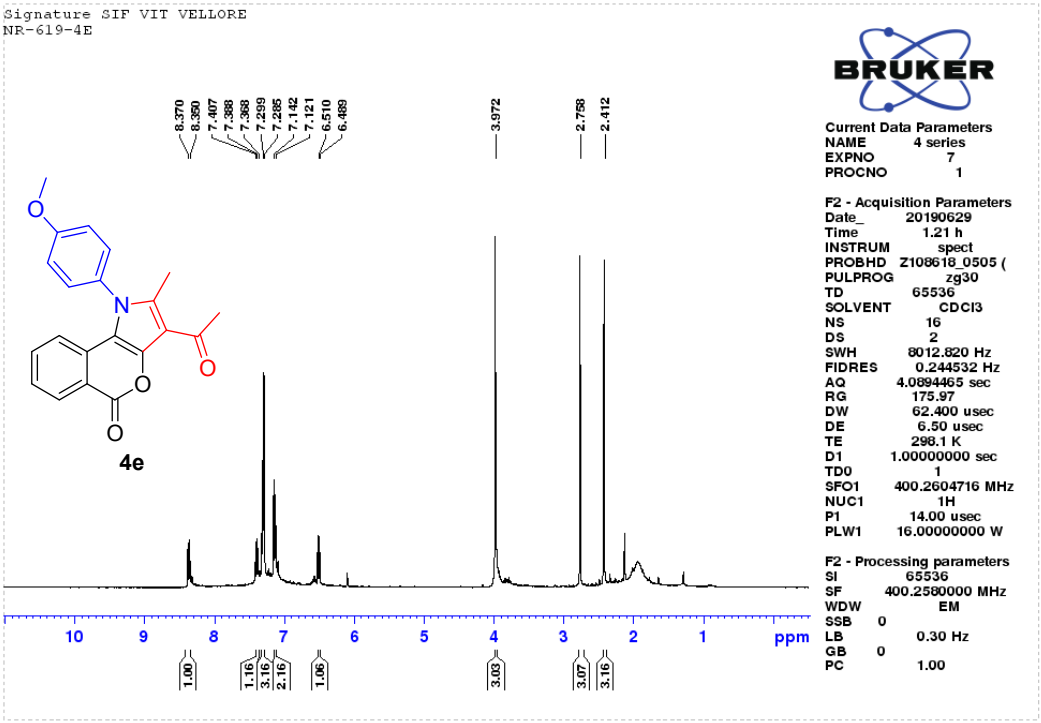


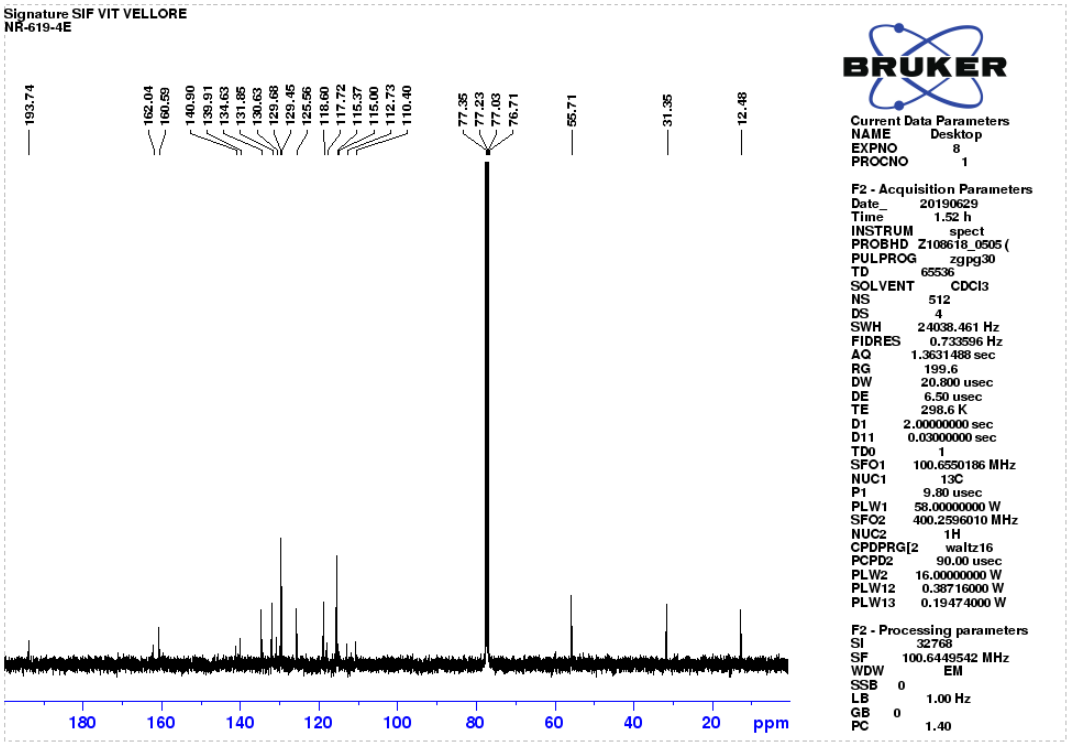
^{1}H &^{13}C Spectrum of 3-acetyl-1-(2,6-diethylphenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4d**



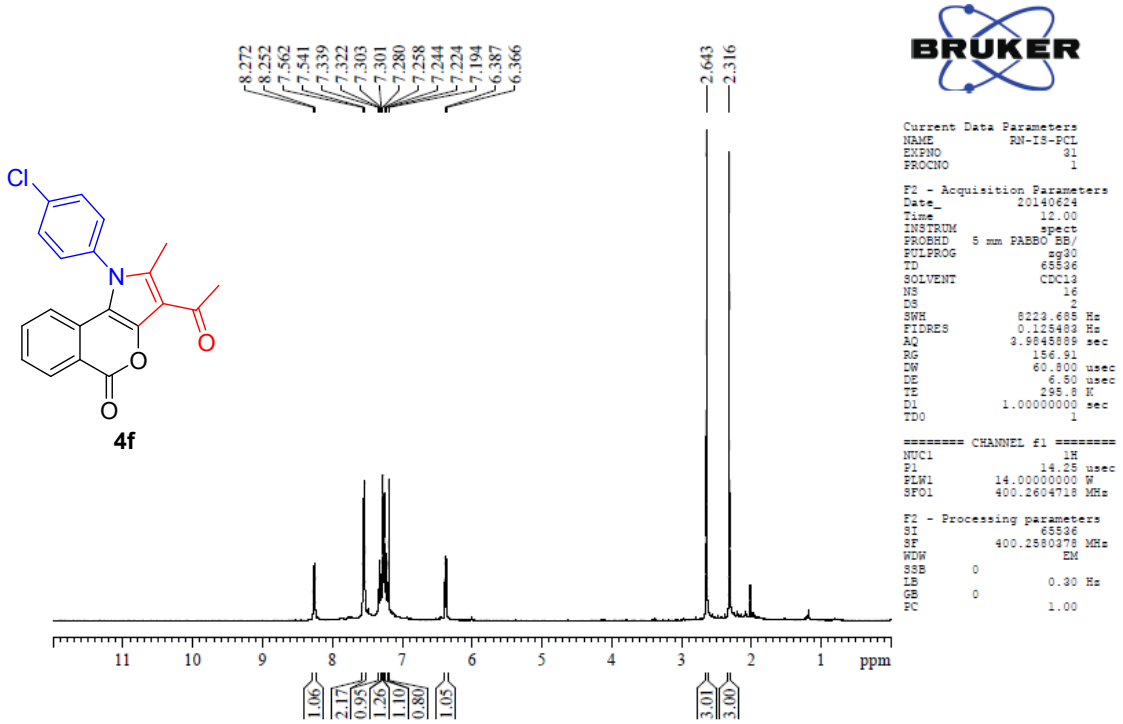


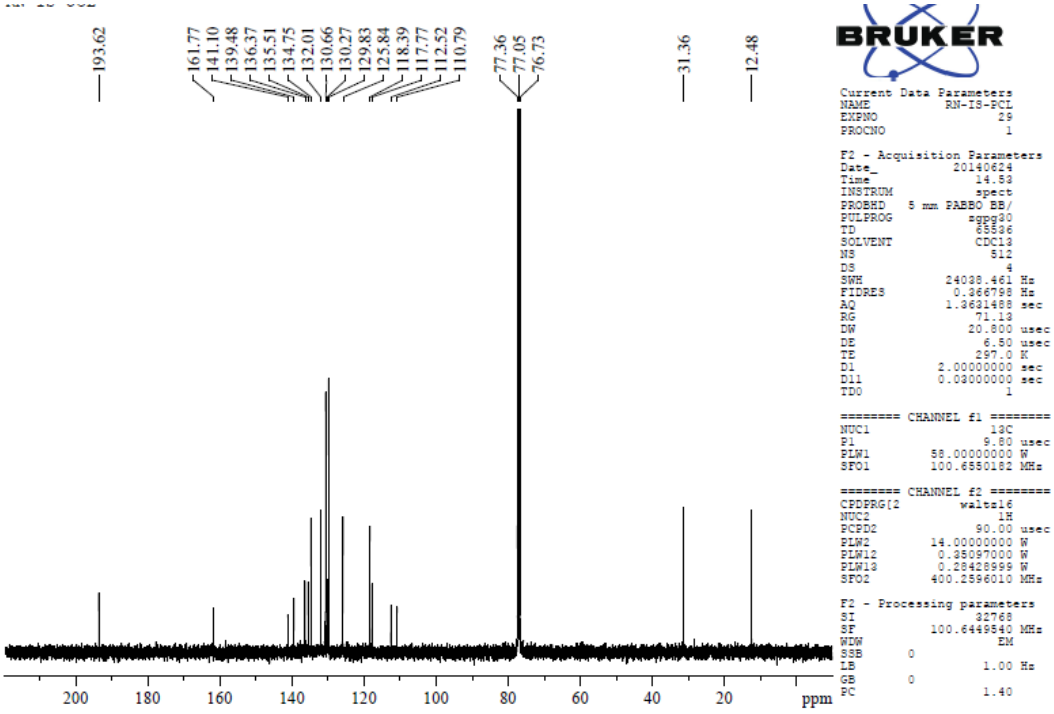
^{1}H &^{13}C spectrum of 3-acetyl-1-(4-methoxyphenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4e**



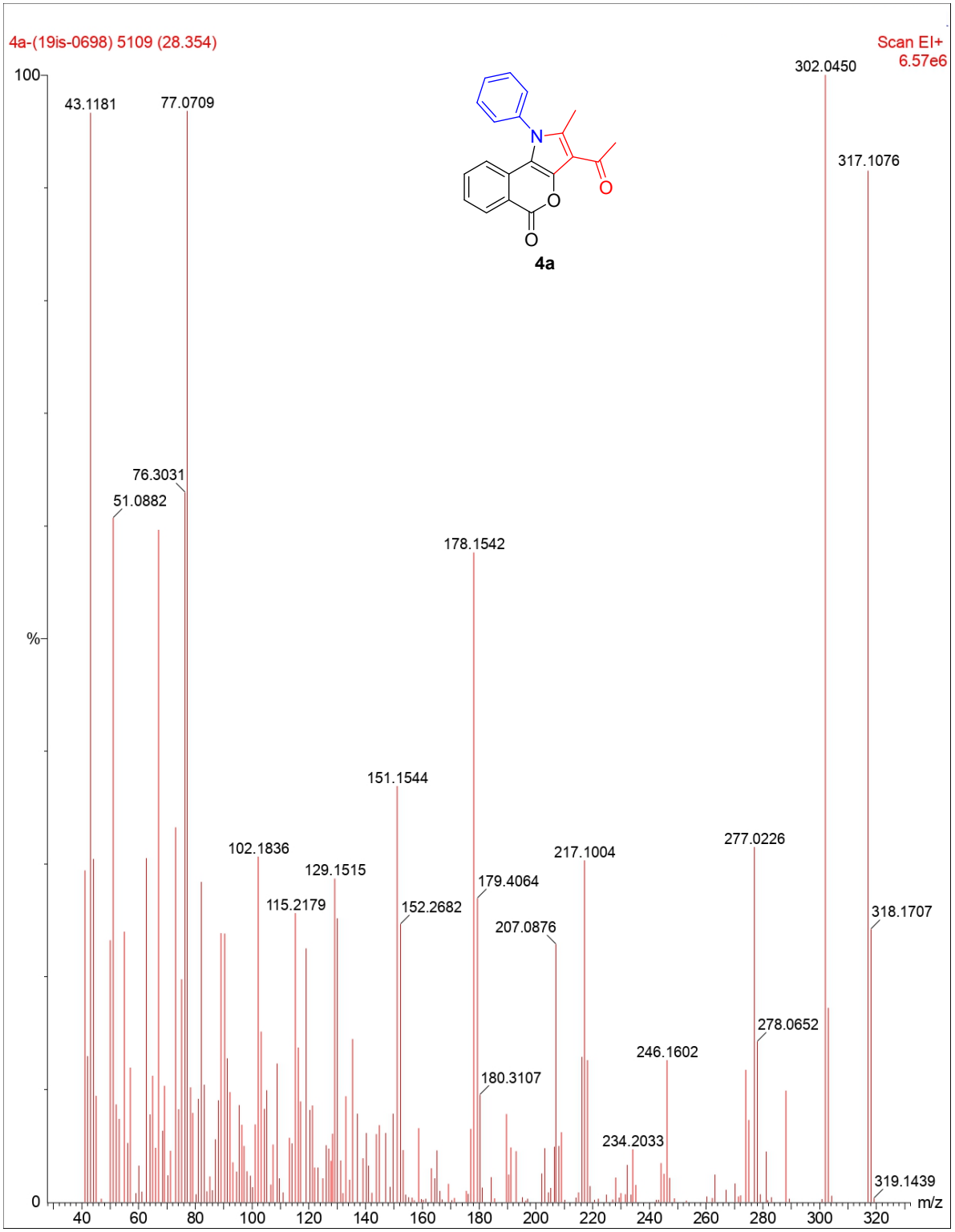


^{1}H &^{13}C NMR Spectrum of 3-acetyl-1-(4-chlorophenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1H)-one, **4f**

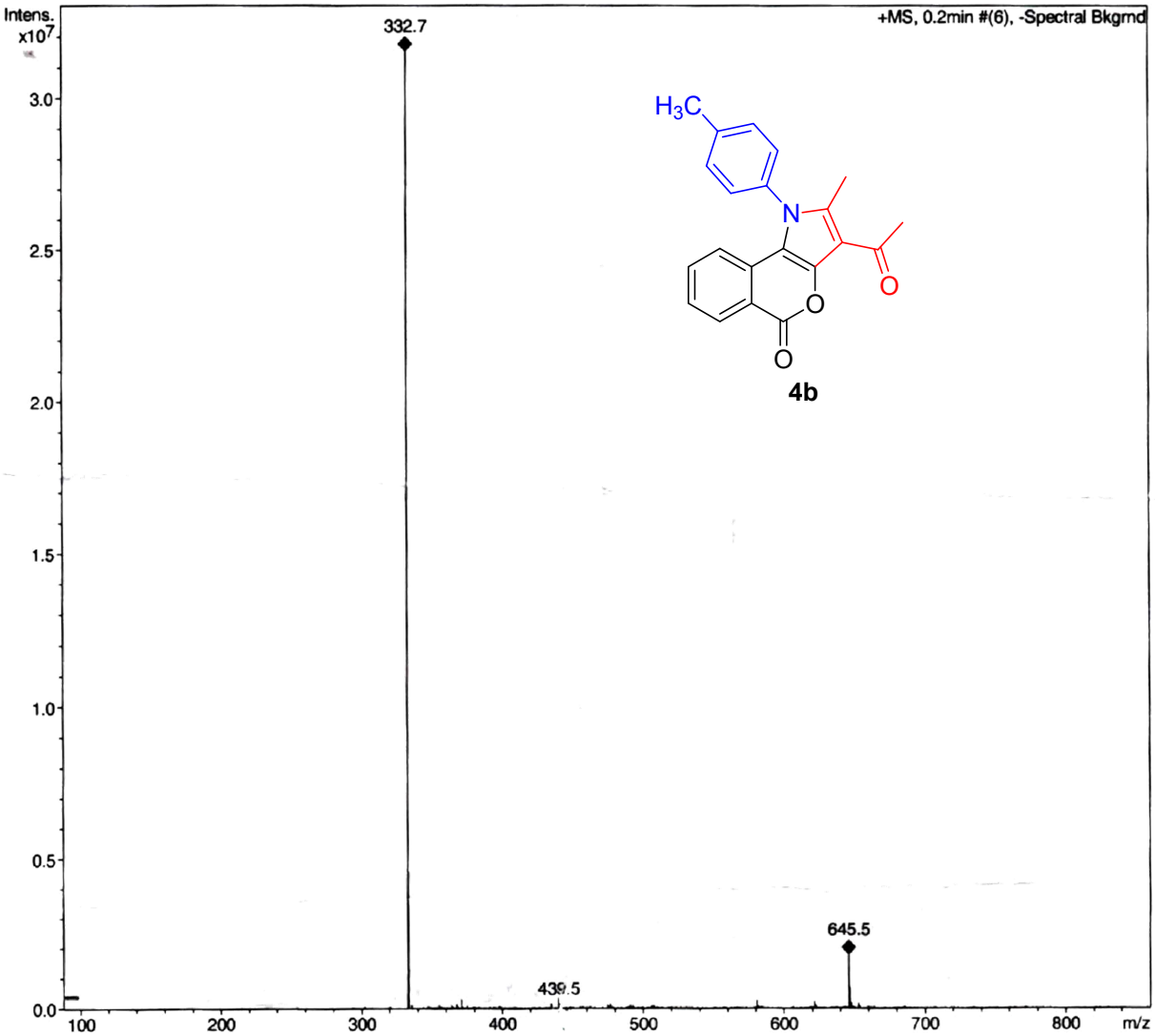


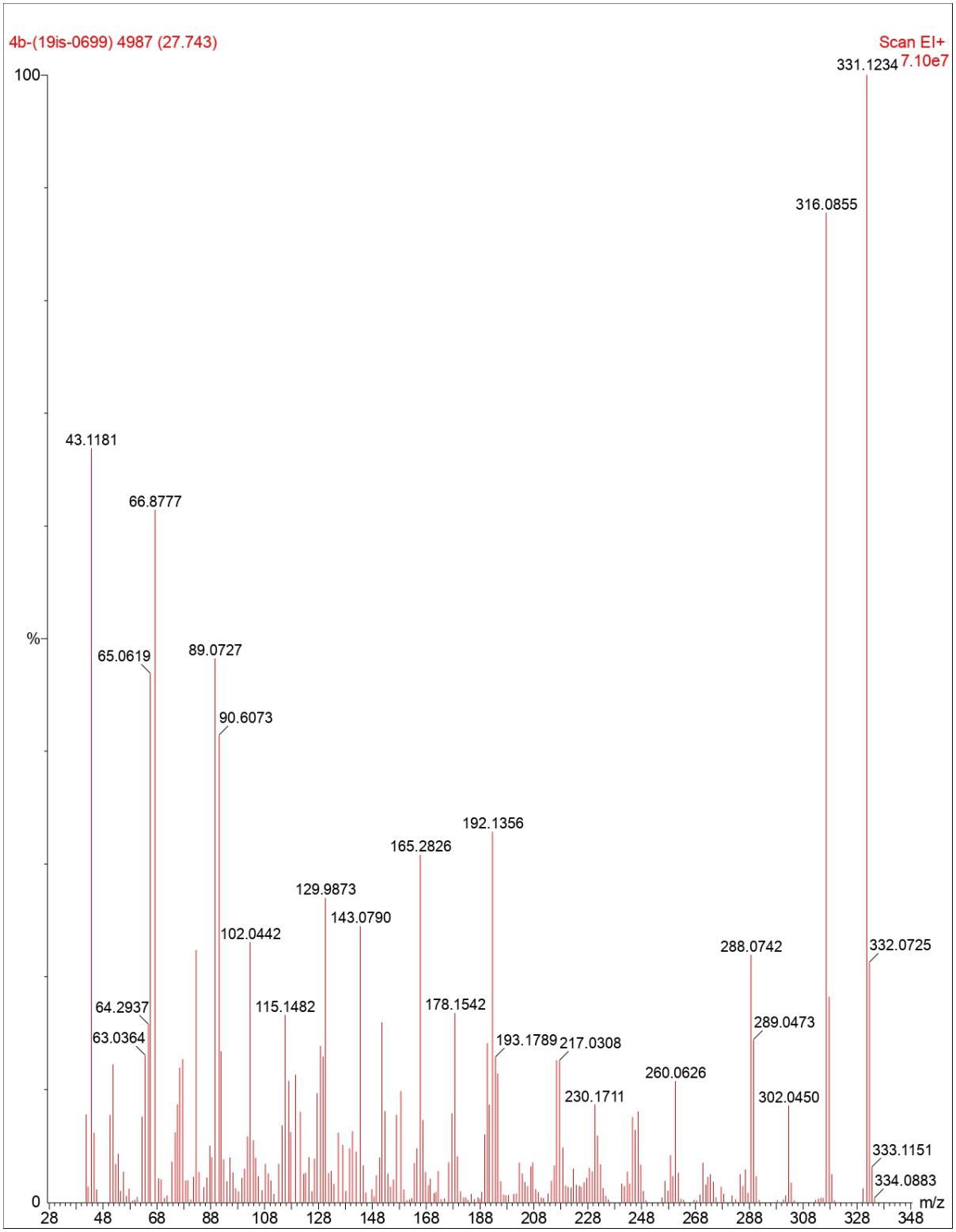


S3: HR-MS Spectrum of 3-acetyl-2-methyl-1-phenylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4a.**



S3. LRMS and HRMS spectrum of 3-acetyl-2-methyl-1-p-tolylisochromeno[4,3-b]pyrrol-5(1*H*)-one **4b.**

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43.1181
66.8777
65.0619
89.0727
90.6073
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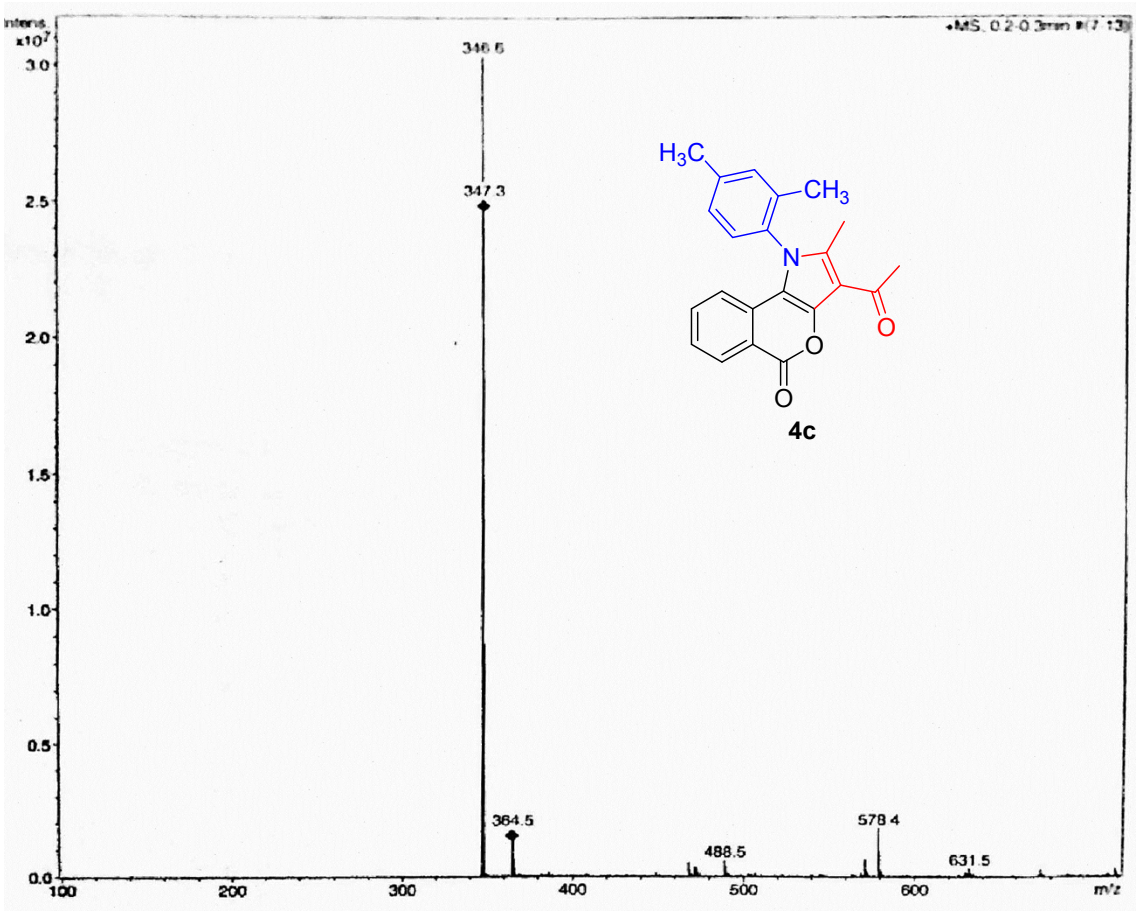
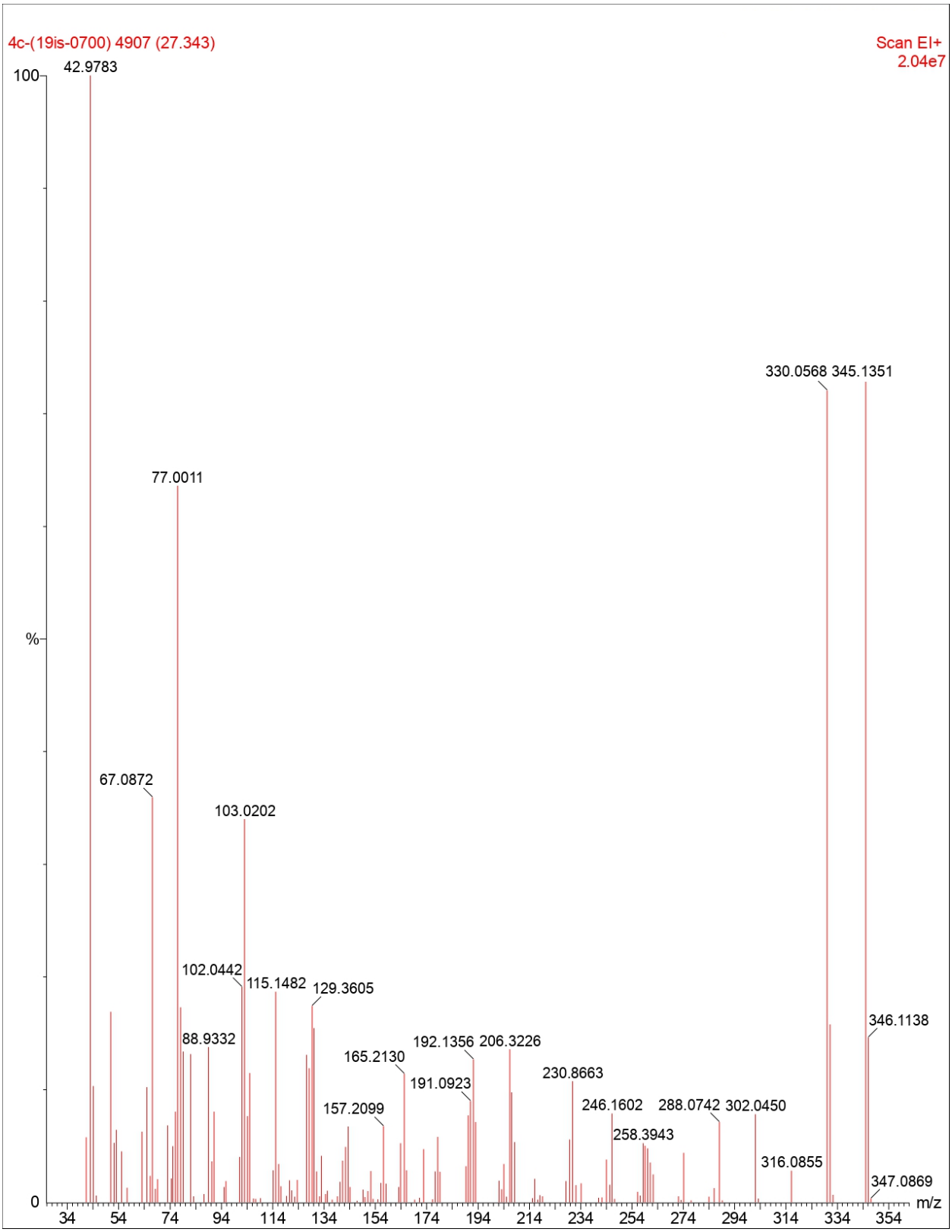
129.9873
143.0790
102.0442
288.0742
332.0725
64.2937
115.1482
178.1542
289.0473
63.0364
193.1789
217.0308
260.0626
230.1711
302.0450
333.1151
334.0883
m/z
28
48
68
88
108
128
148
168
188
208
228
248
268
288
308
328
348

S3: LRMS and HRMS Spectrum of 3-acetyl-2-methyl-1-(2,4-dimethylphenyl)isochromeno[4,3-b]pyrrol-5(1*H*)-one, **4c**

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102.0442
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230.8663
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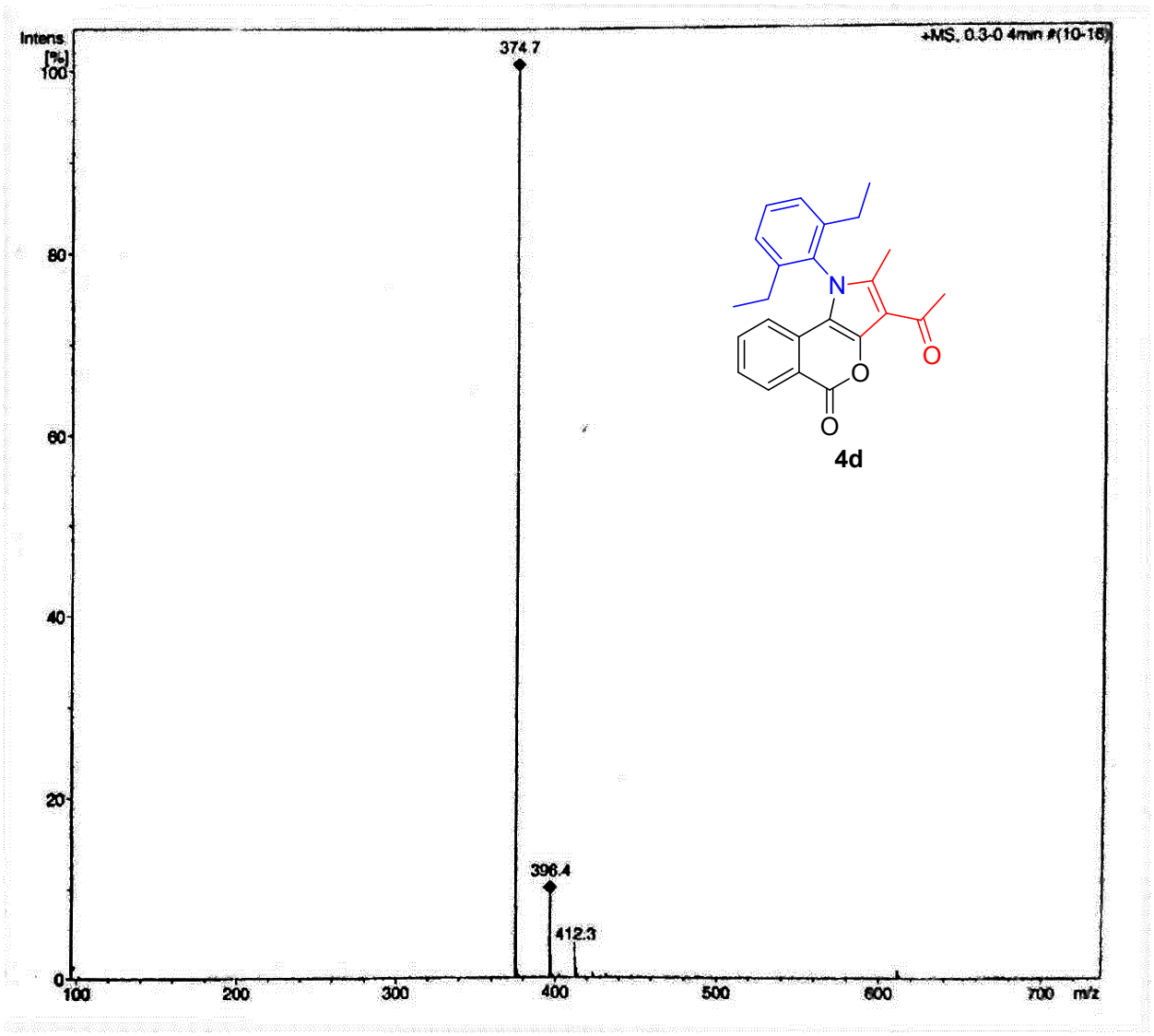
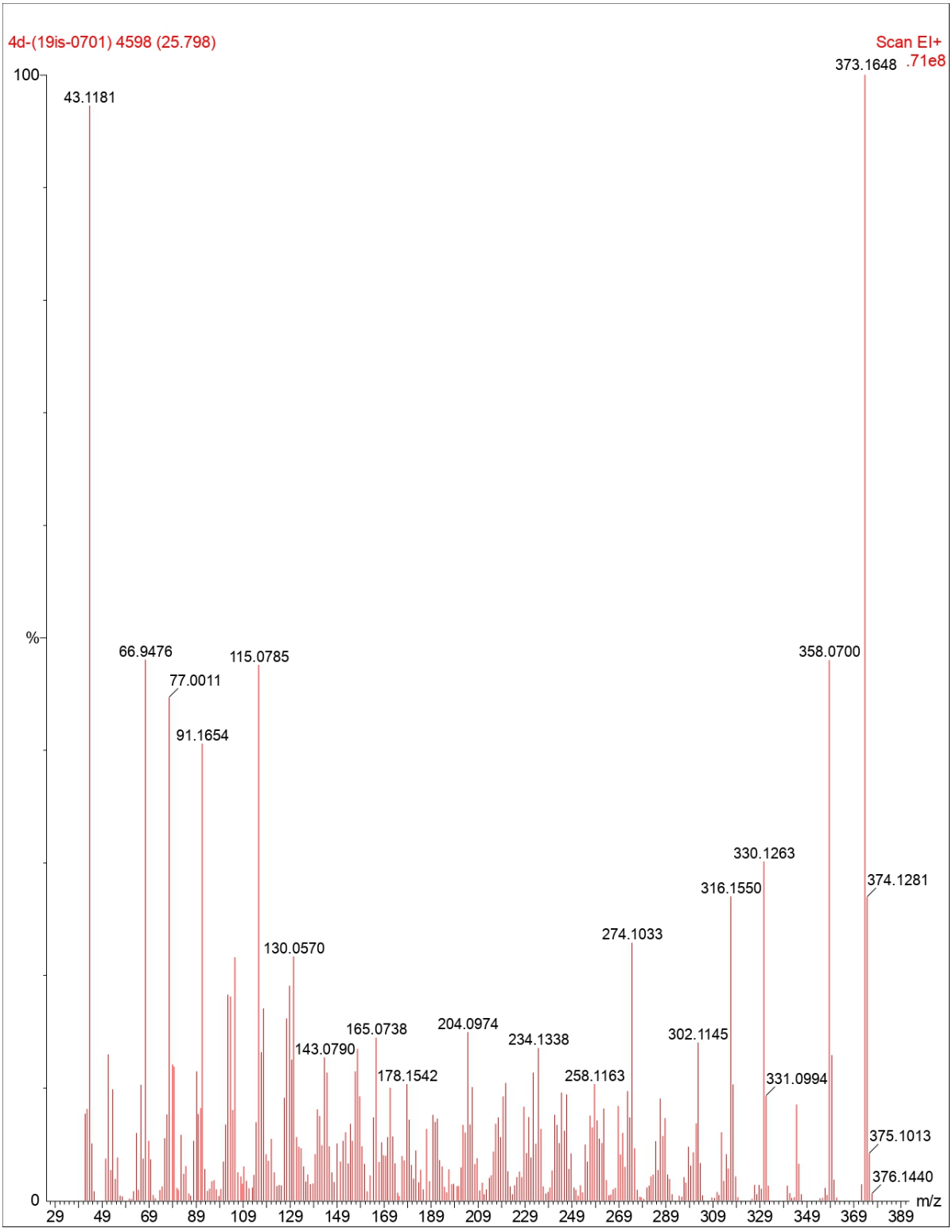
302.0450
258.3943
316.0855
330.0568
345.1351
346.1138
347.0869
34
54
74
94
114
134
154
174
194
214
234
254
274
294
314
334
354
m/z

S3: LRMS and HRMS Spectrum of 3-acetyl-1-(2,6-diethylphenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4d**

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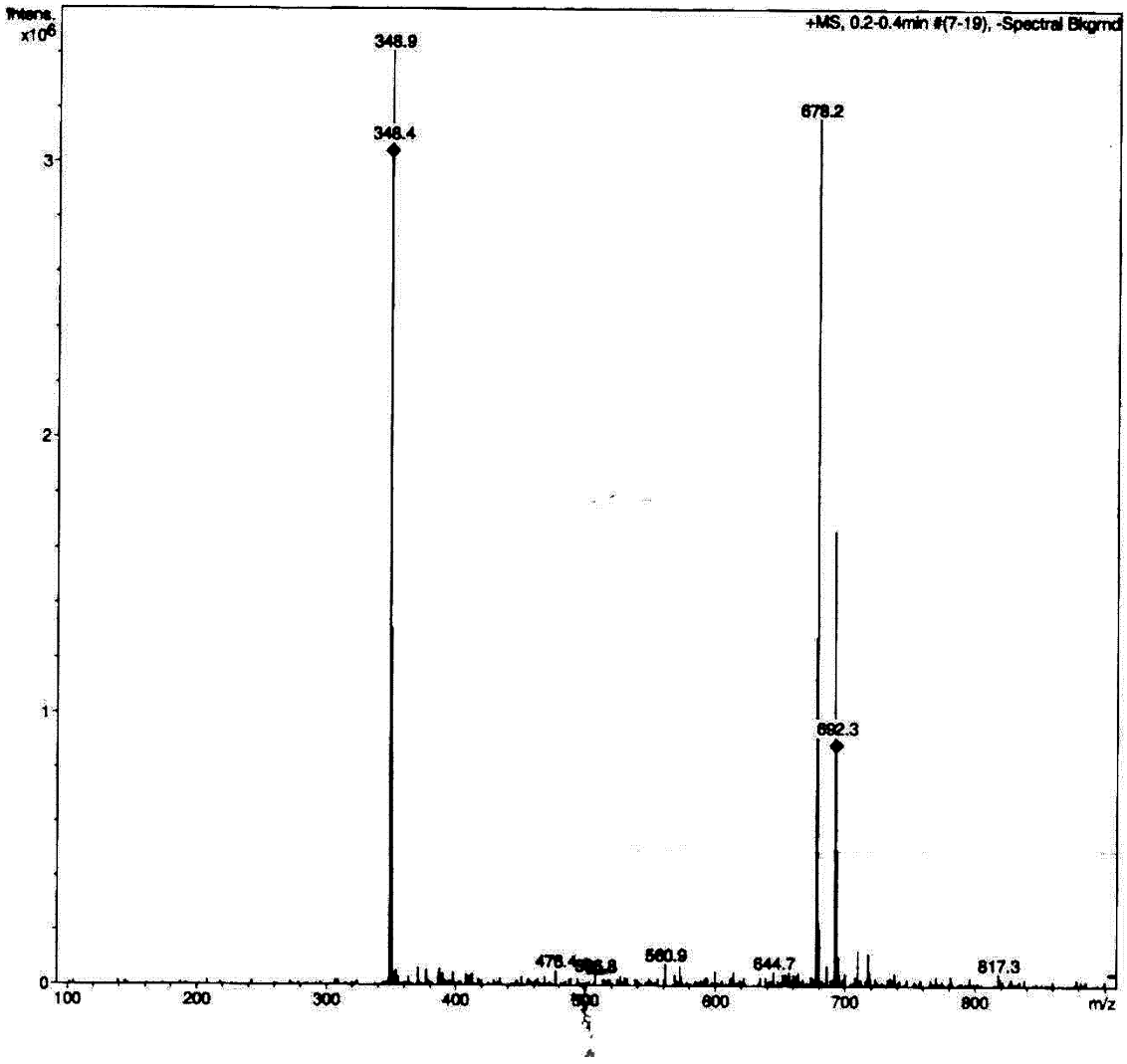
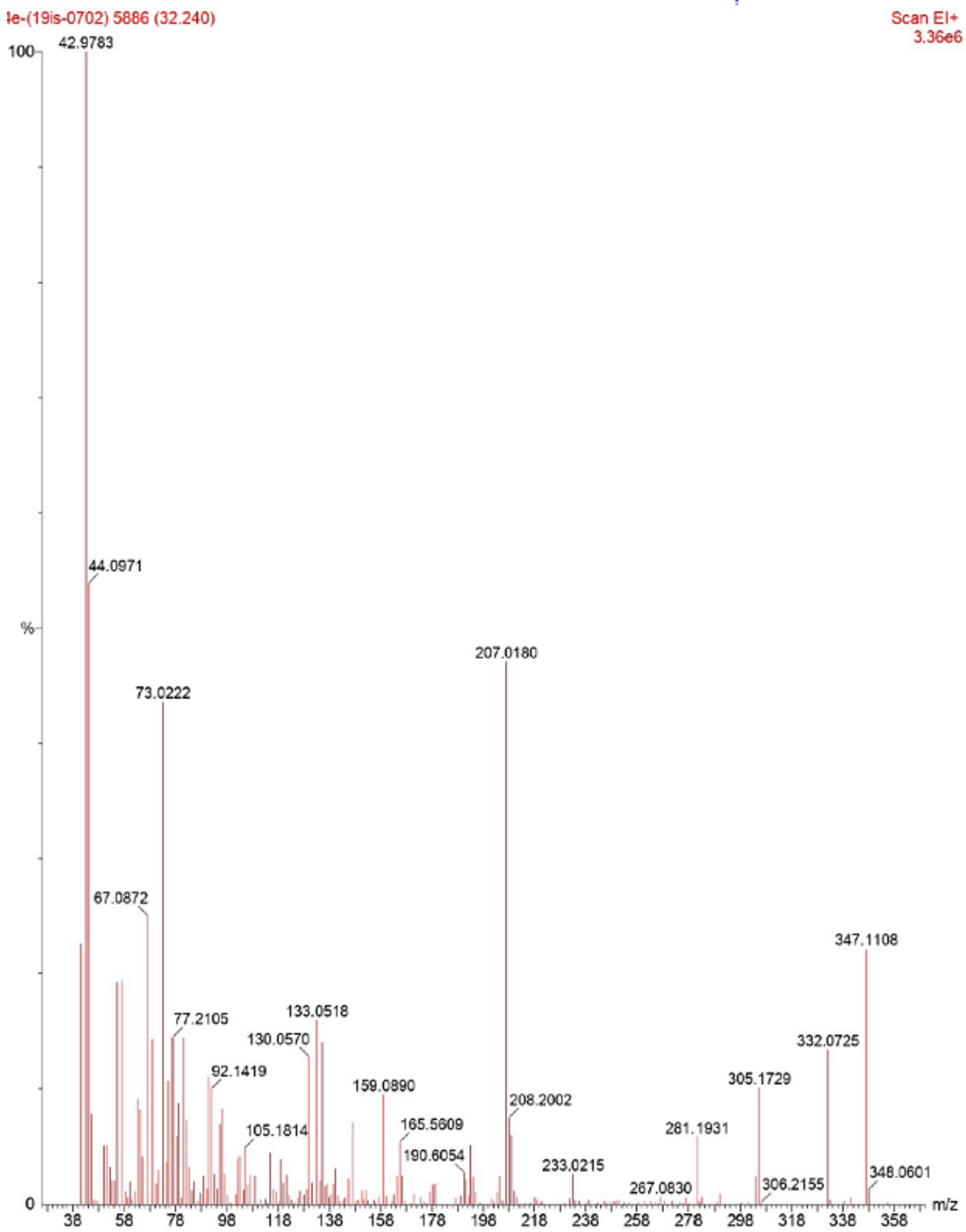
66.9476
115.0785
77.0011
91.1654
358.0700
330.1263
316.1550
374.1281
274.1033
130.0570
165.0738
204.0974
234.1338
143.0790
302.1145
178.1542
258.1163
331.0994
375.1013
376.1440
29 49 69 89 109 129 149 169 189 209 229 249 269 289 309 329 349 369 389
m/z

S3: LRMS and HRMS spectrum of 3-acetyl-1-(4-methoxyphenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1*H*)-one, **4e**

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%
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77.2105
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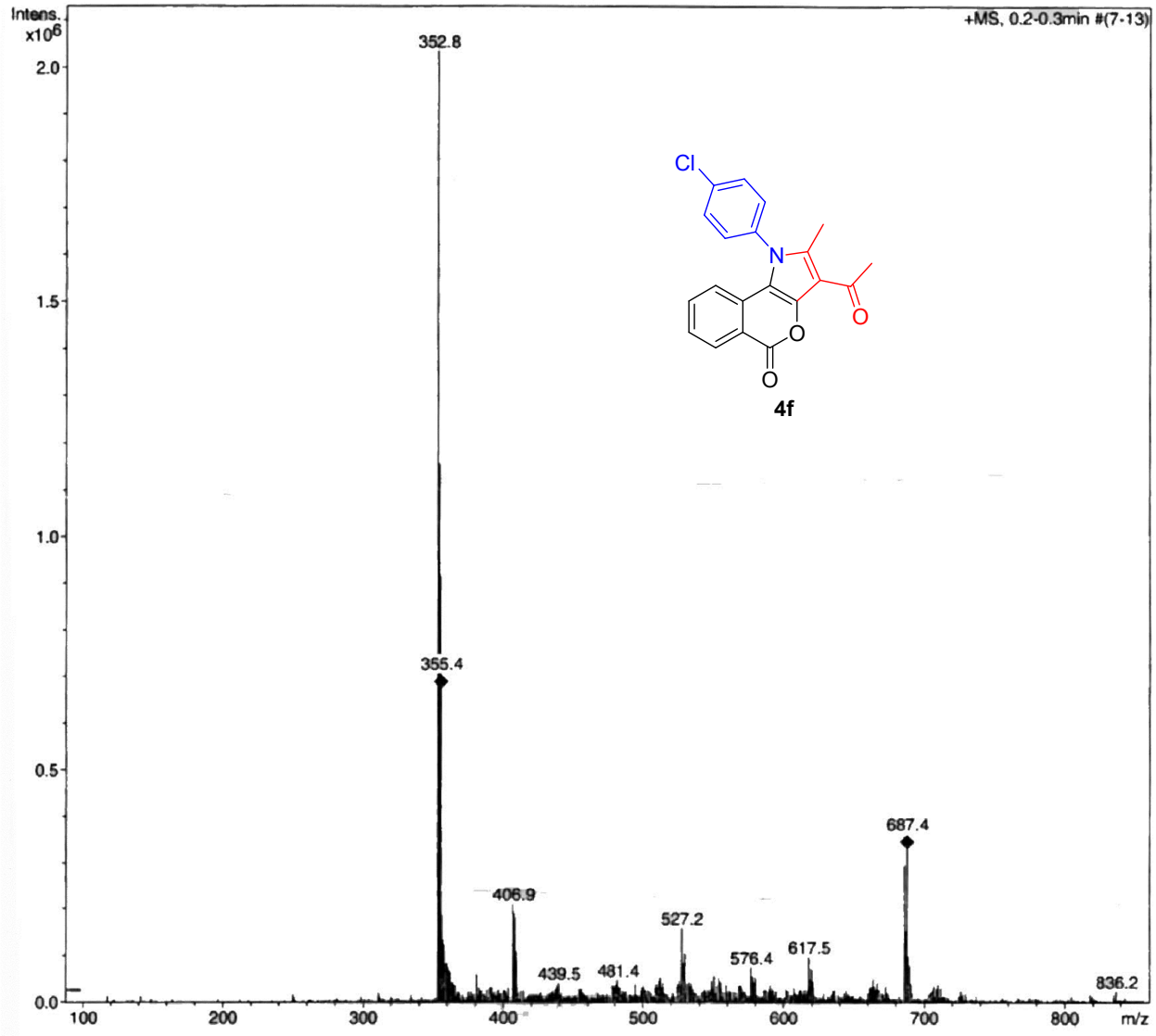
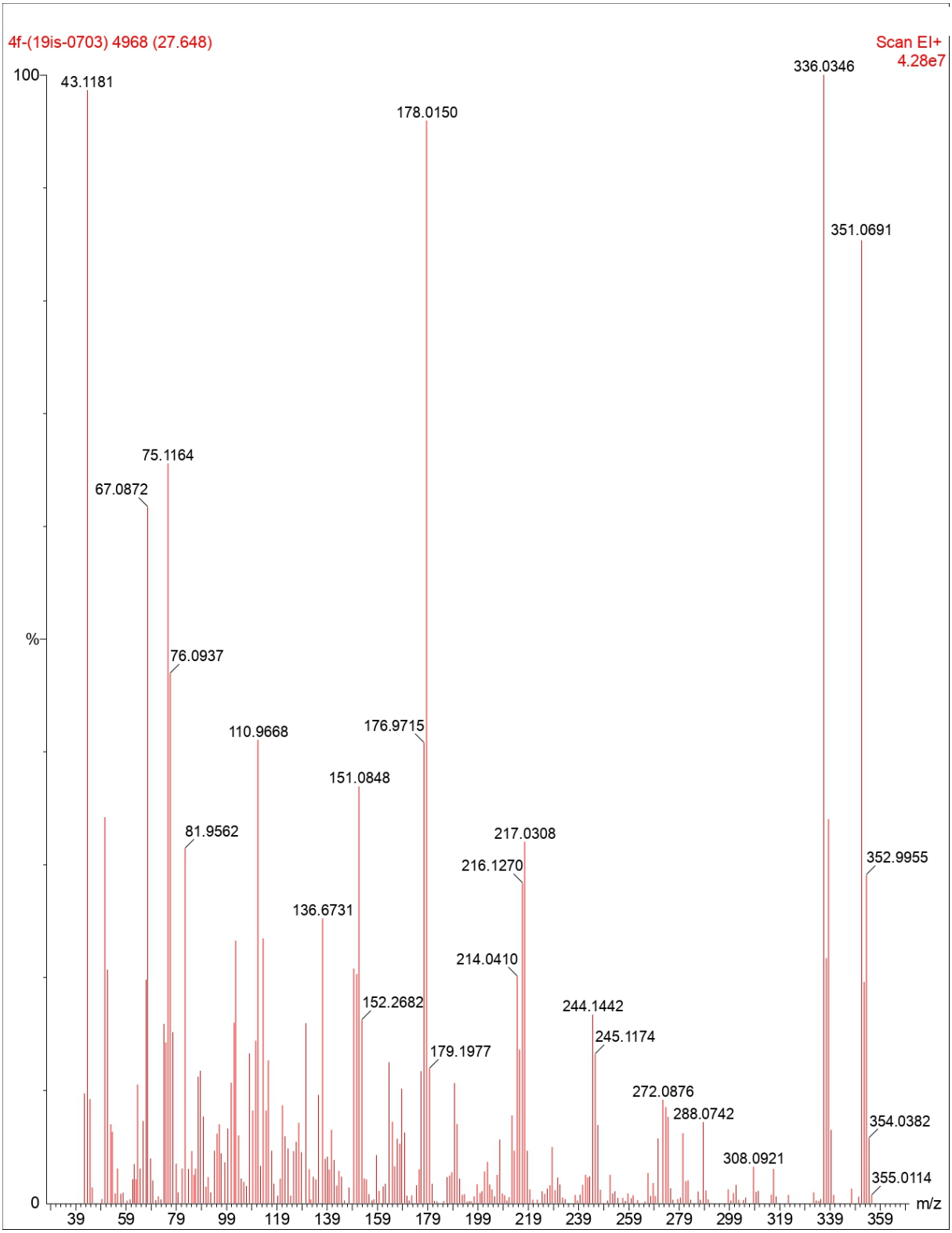
332.0725
92.1419
305.1729
159.0890
208.2002
165.5609
281.1931
105.1814
190.6054
233.0215
348.0601
267.0830
306.2155
m/z
38
58
78
98
118
138
158
178
198
218
238
258
278
298
318
338
358

S3: LRMS and HRMS Spectrum of 3-acetyl-1-(4-chlorophenyl)-2-methylisochromeno[4,3-b]pyrrol-5(1H)-one, **4f**

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Scan EI+
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100
%
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178.0150
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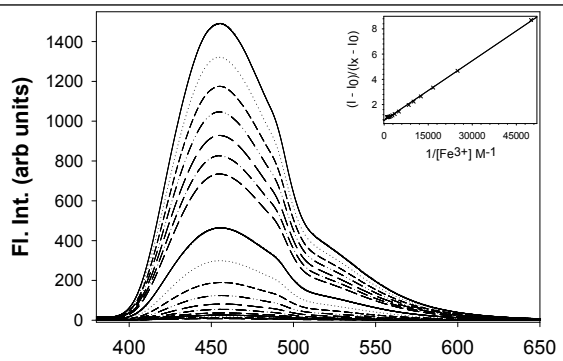
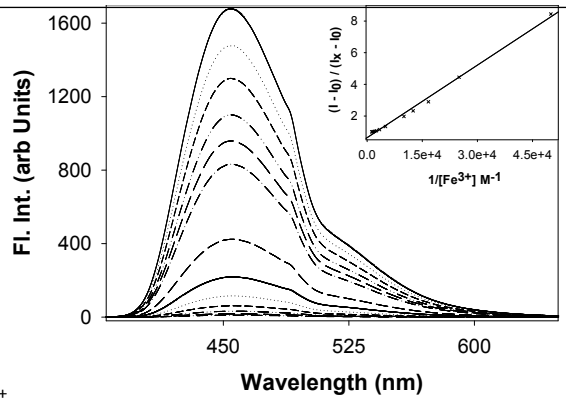
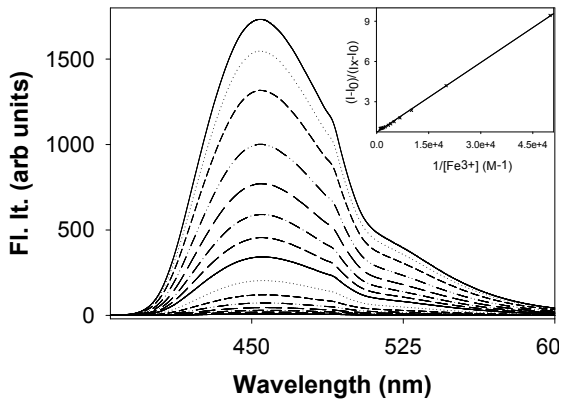
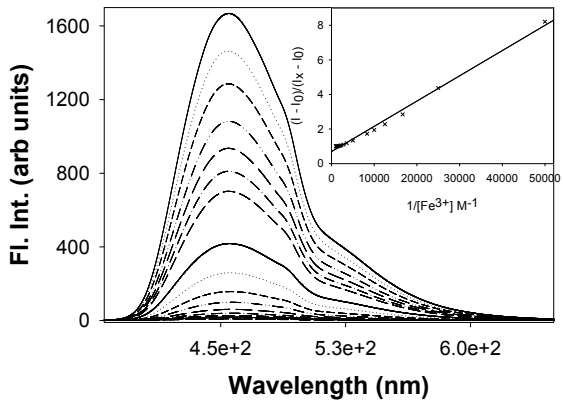
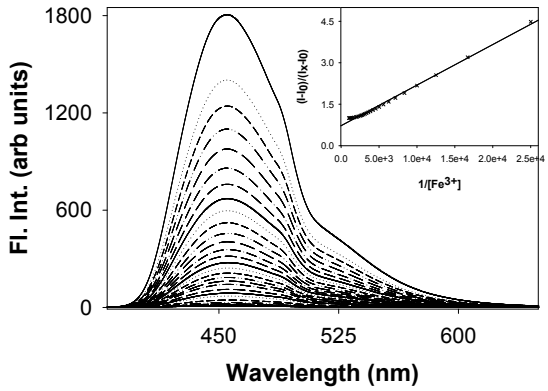
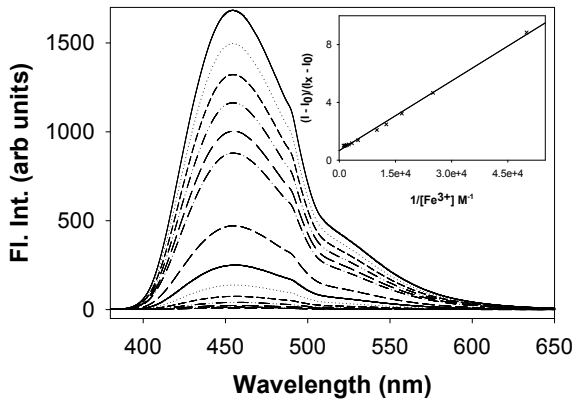
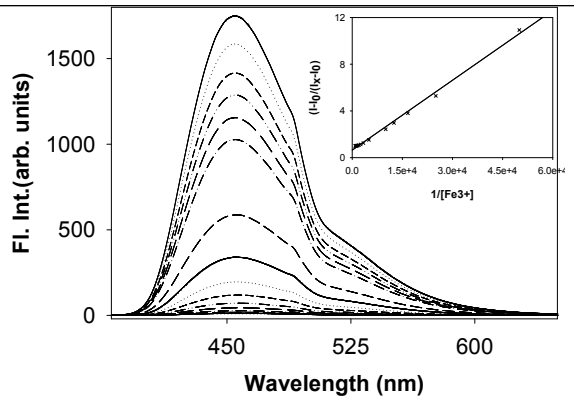
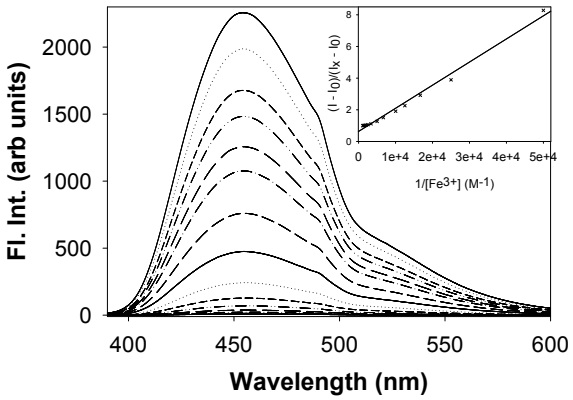
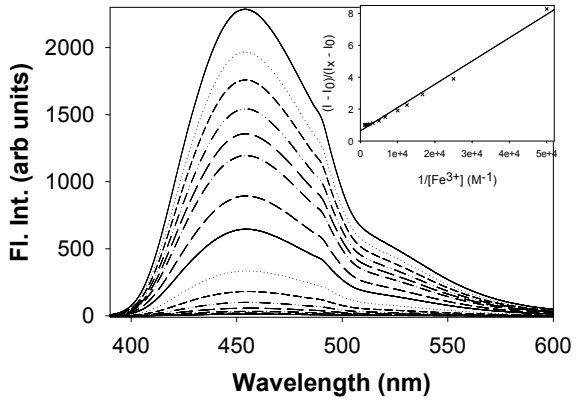
176.9715
151.0848
81.9562
217.0308
216.1270
352.9955
136.6731
214.0410
152.2682
244.1442
245.1174
179.1977
272.0876
288.0742
354.0382
308.0921
355.0114
39
59
79
99
119
139
159
179
199
219
239
259
279
299
319
339
359
m/z

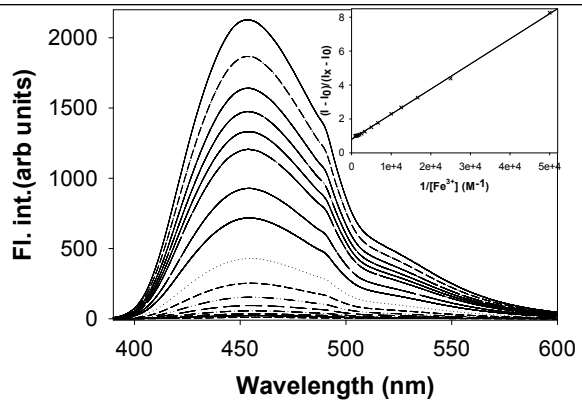
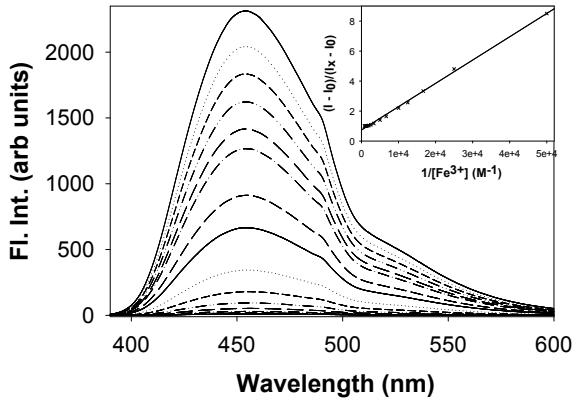
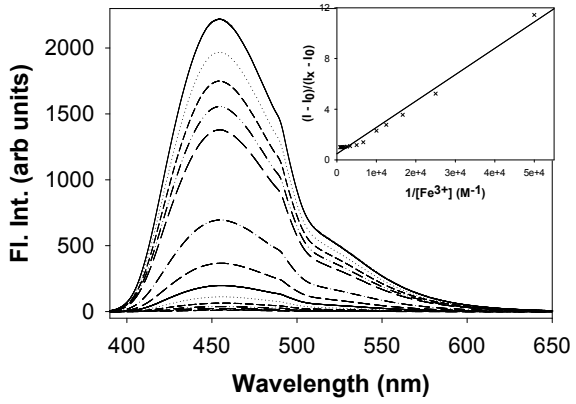
S4: Fluorescence turn-off sensing of Fe(III) in the presence of other metal ions and their association constants

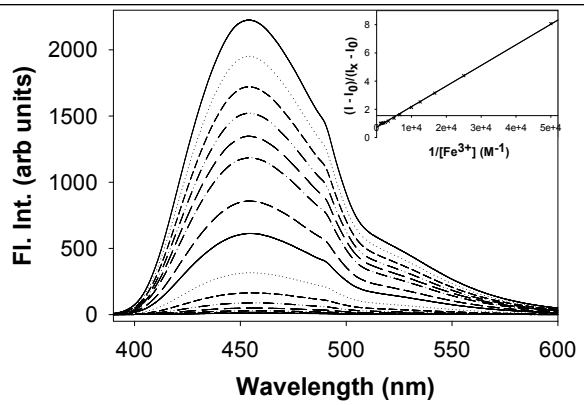
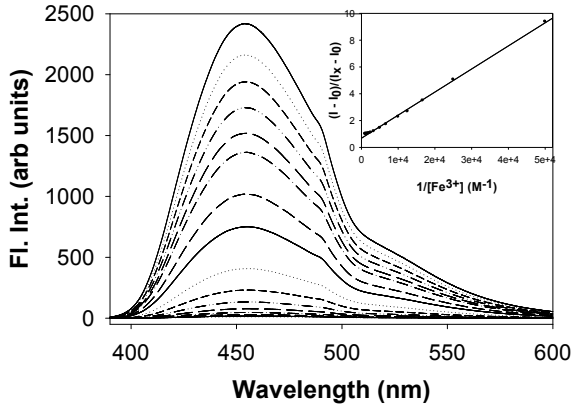
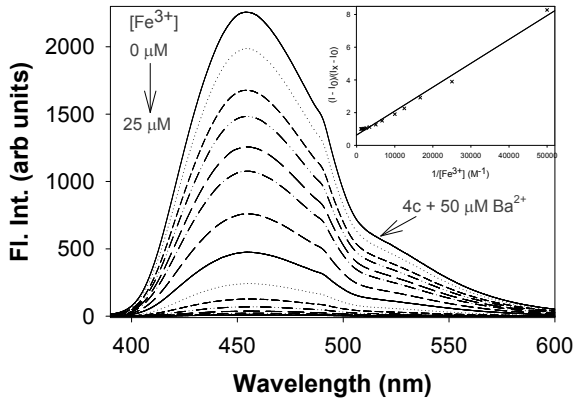
Sensing of metal ions:

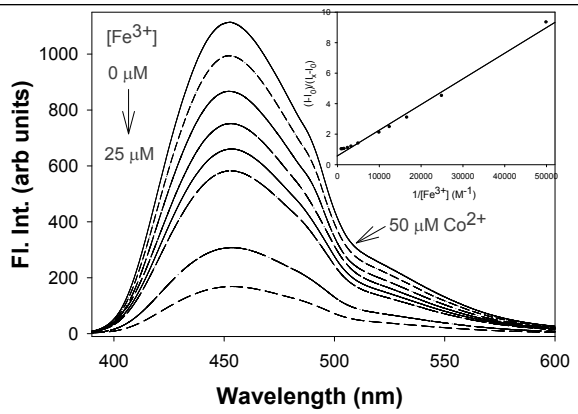
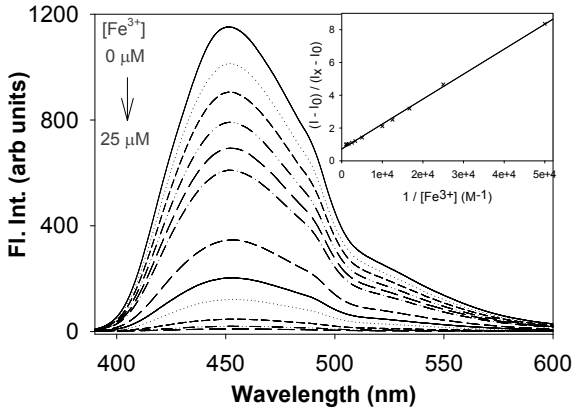
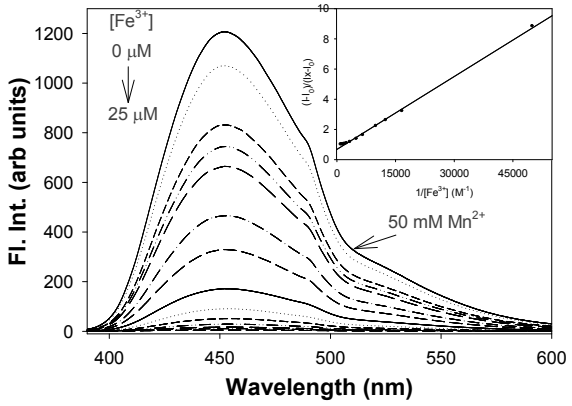
Compound	Quenching by Fe^{3+}	Ka (M^{-1})
4a	 Ba^{2+}	4.75×10^3
	 Co^{2+}	4.157×10^3
	Fe^{3+} 	4.14×10^3

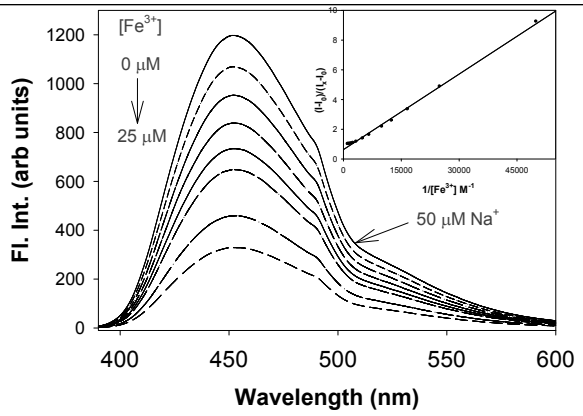
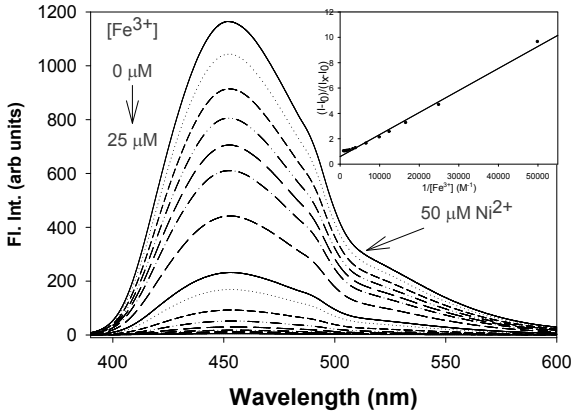
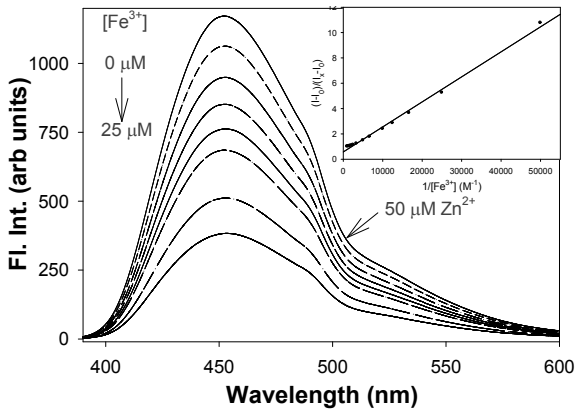
	Mn^{2+} 	4.74×10^3
	Na^{+} 	4.95×10^3
	Ni^{2+} 	4.16×10^3
	Zn^{2+}	3.22×10^3

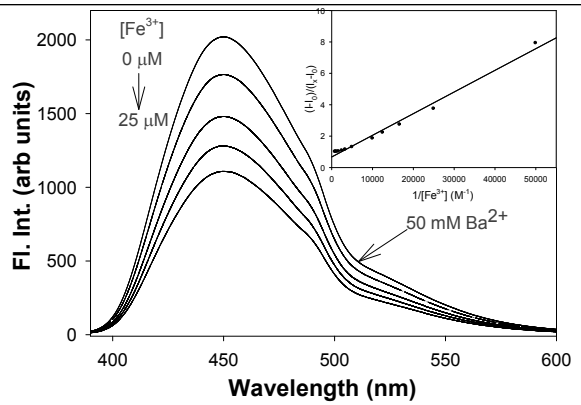
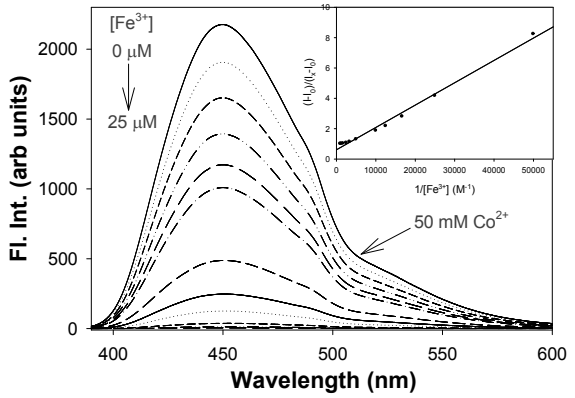
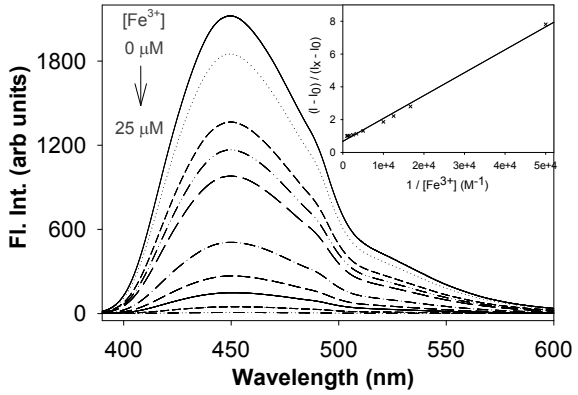
		
4b	Ba^{2+} 	4.34×10^3
	Co^{2+} 	4.35×10^3
	Fe^{3+}	5.39×10^3

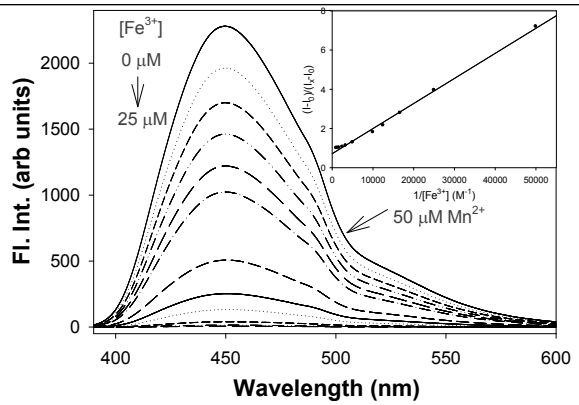
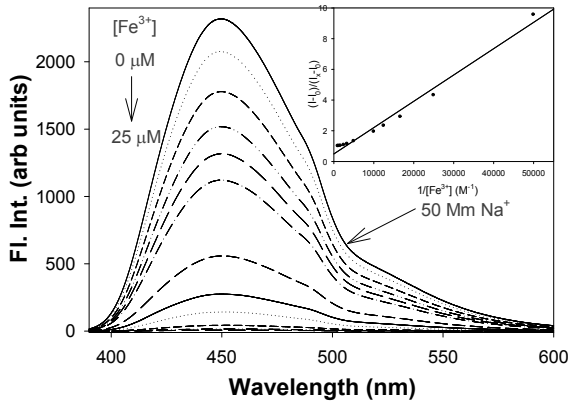
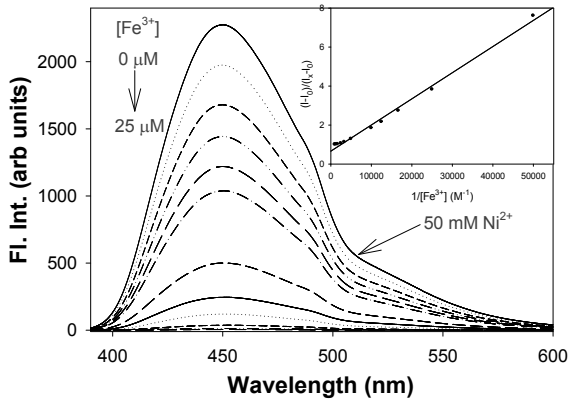
		
	Mn^{2+} 	4.76×10^3
	Na^{+} 	2.30×10^3
	Ni^{2+}	4.98×10^3

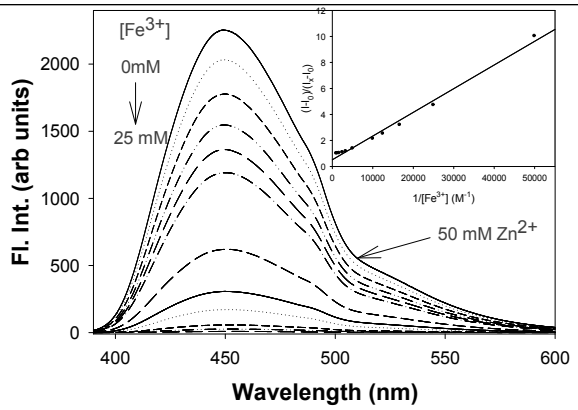
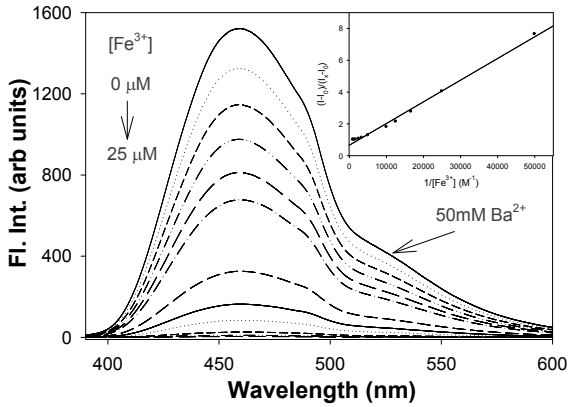
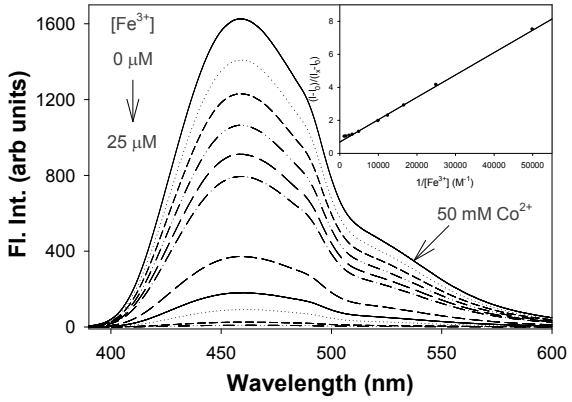
		
	Zn^{2+} 	3.98×10^3
4c	Ba^{2+} 	4.35×10^3
	Co^{2+}	3.46×10^3

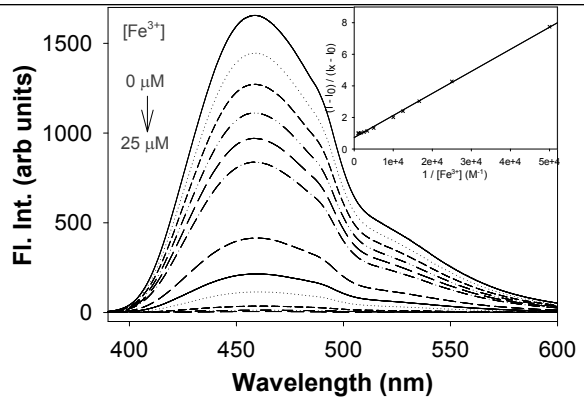
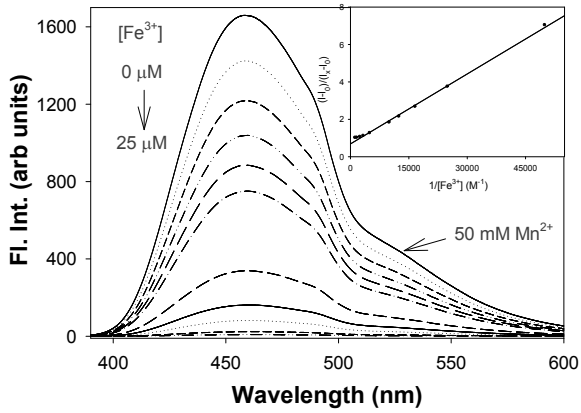
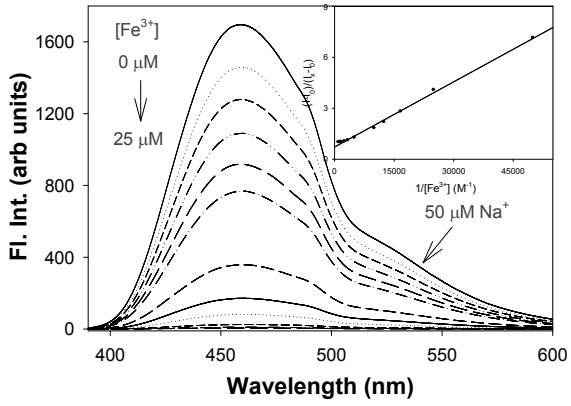
		
	Fe^{3+} 	4.74×10^3
	Mn^{2+} 	4.20×10^3
	Na^{+}	3.74×10^3

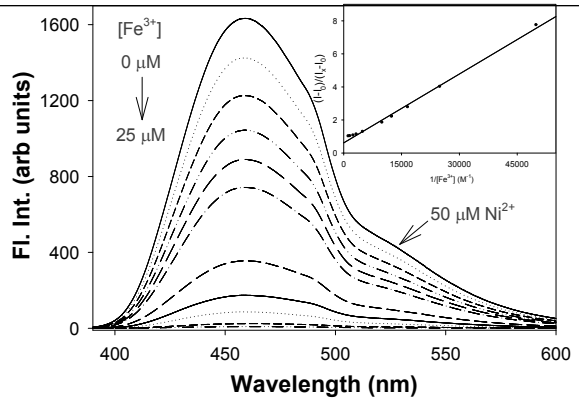
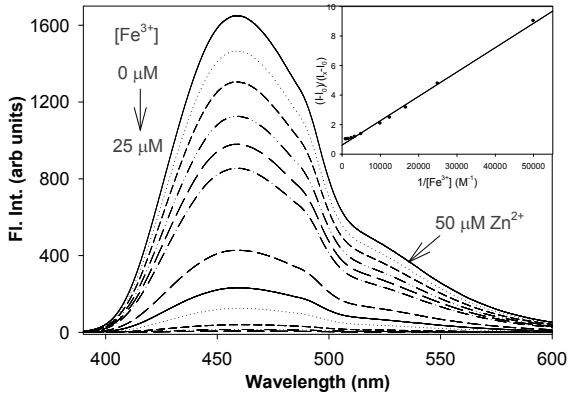
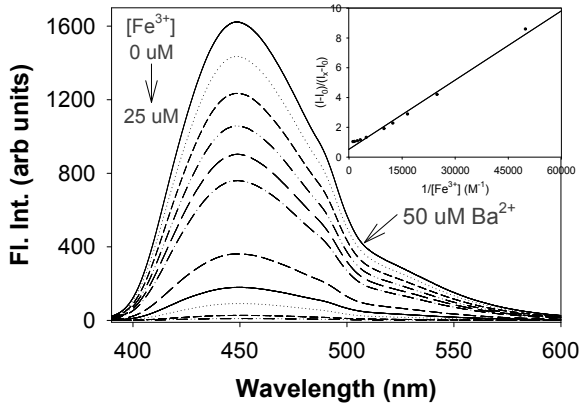
		
	Ni^{2+} 	3.40×10^3
	Zn^{2+} 	2.93×10^3
4d	Ba^{2+}	4.87×10^3

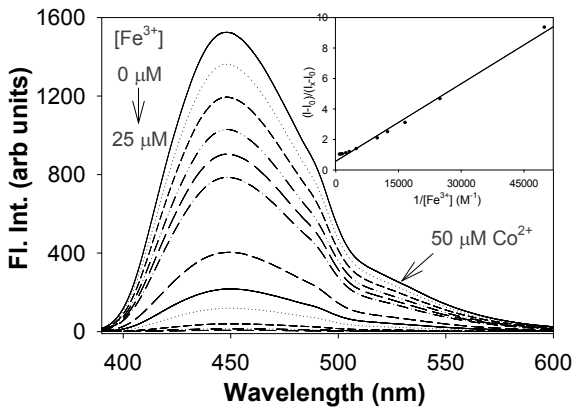
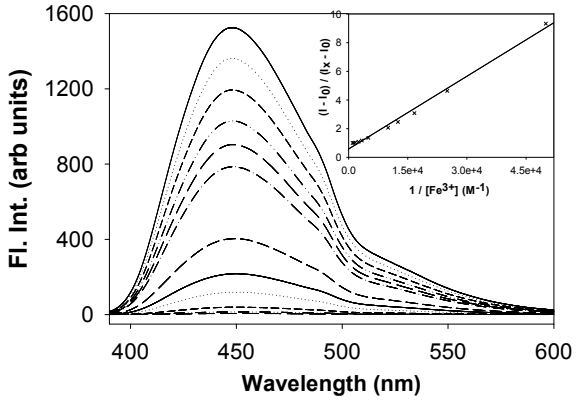
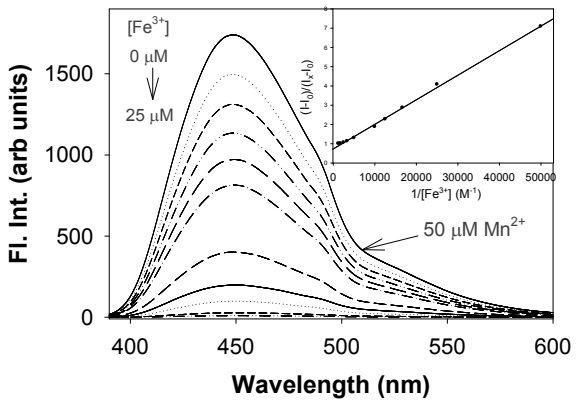
		
	Co^{2+} 	4.15×10^3
	Fe^{3+} 	4.81×10^3
	Mn^{2+}	5.59×10^3

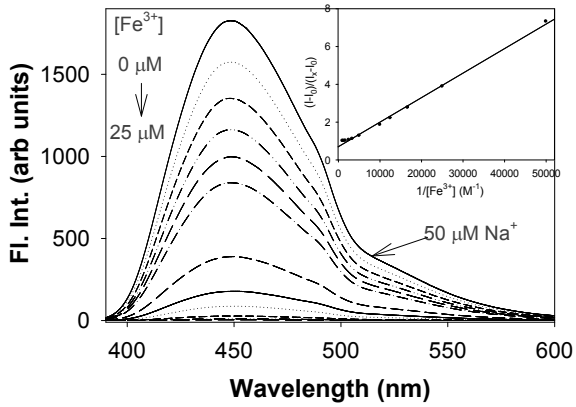
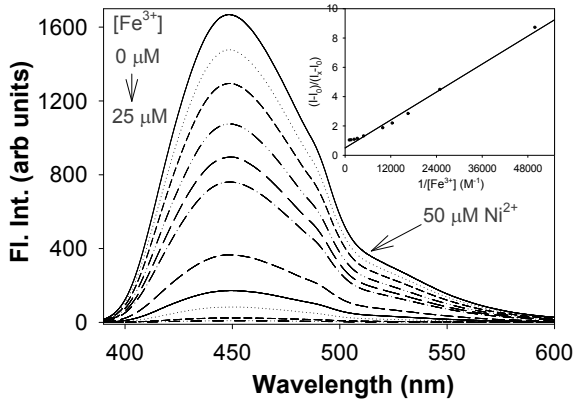
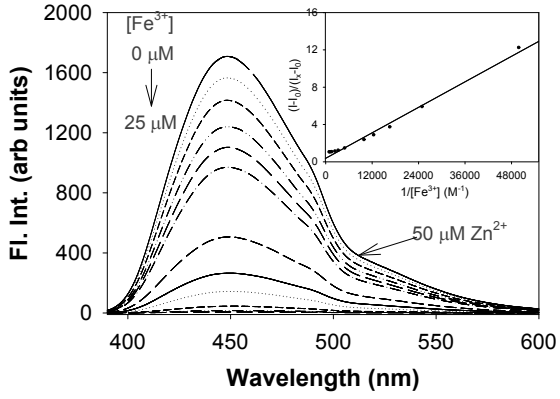
		
	Na^+ 	5.03×10^3
	Ni^{2+} 	6.69×10^3
	Zn^{2+}	2.85×10^3

		
4e	Ba^{2+} 	4.83 x 10^3
	Co^{2+} 	5.09 x 10^3
	Fe^{3+}	5.20 x 10^3

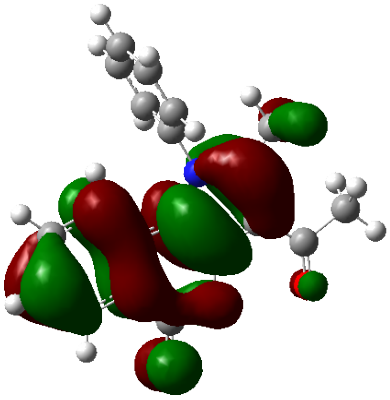
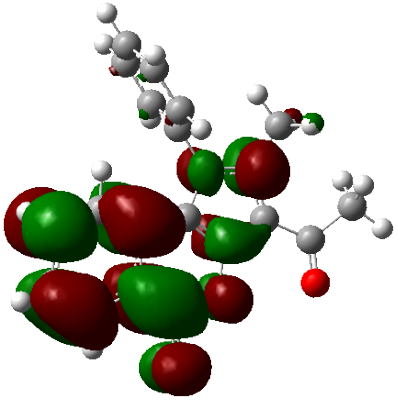
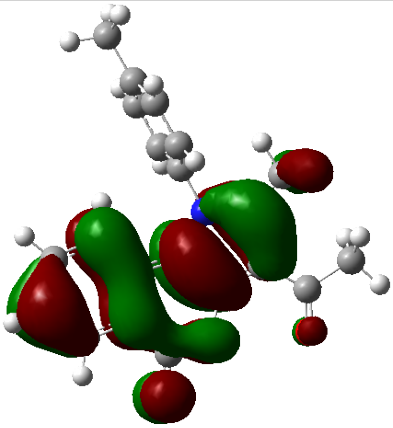
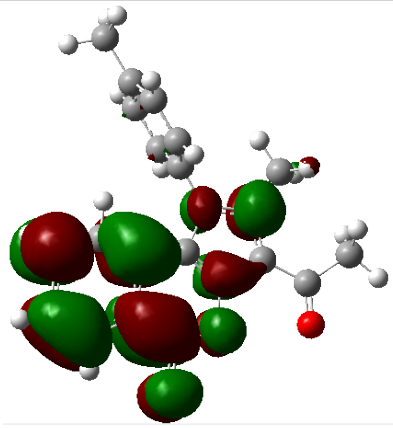
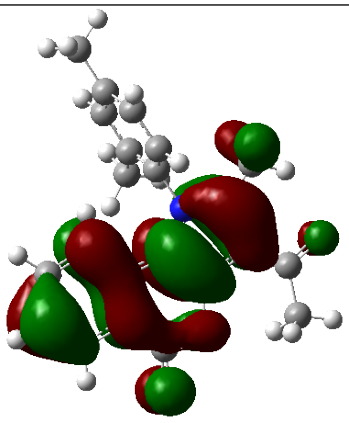
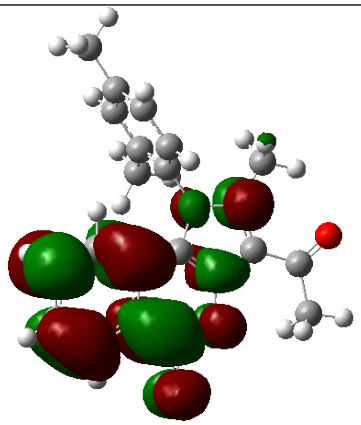
		
	Mn^{2+} 	5.49×10^3
	Na^{+} 	6.65×10^3
	Ni^{2+}	6.21×10^3

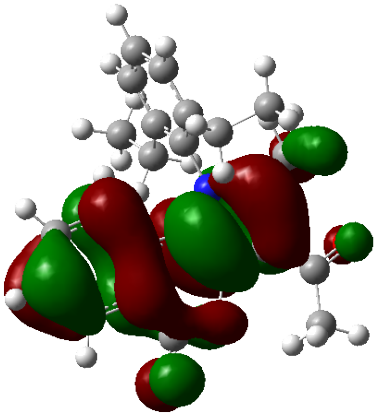
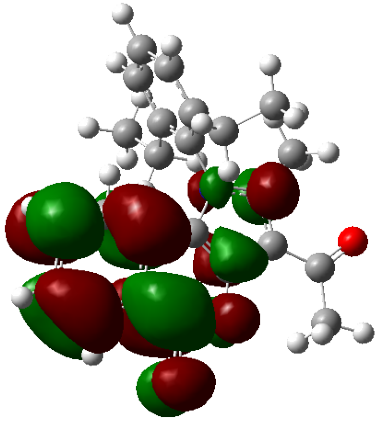
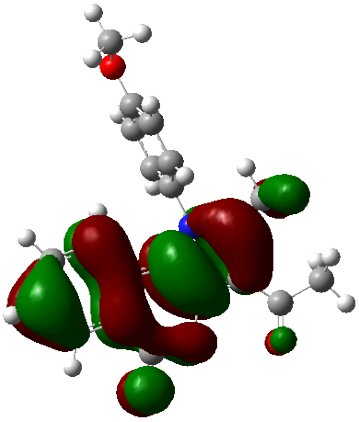
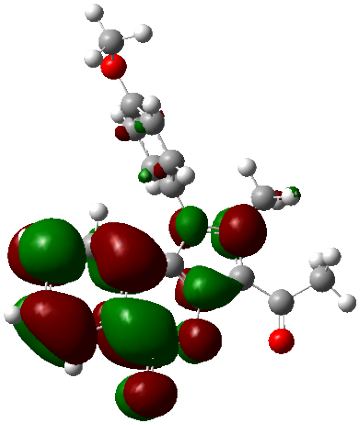
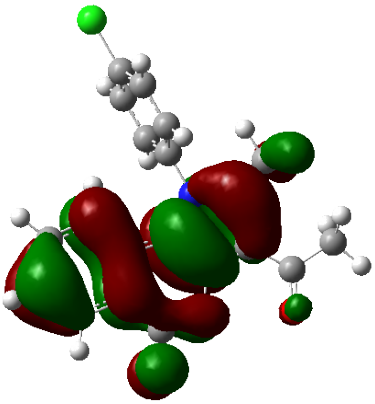
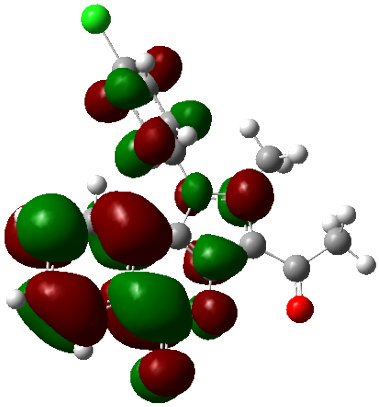
		
	Zn^{2+} 	3.74×10^3
4f	Ba^{2+} 	3.42×10^3
	Co^{2+}	5.82×10^3

		
	Fe^{3+} 	5.82×10^3
	Mn^{2+} 	7.32×10^3

	Na^+ 	5.41×10^3
	Ni^{2+} 	3.17×10^3
	Zn^{2+} 	1.68×10^3

S5: Molecular orbital diagram for the HOMO and LUMO of **4a–f** along with transition energy in eV.

	HOMO	**LUMO**	**ΔE (eV)**
4a			-6.78
4b			-6.69
4c			-6.75

4d			-6.75
4e			-6.67
4f			-6.86

S6: Ground and Excited state geometry optimized molecular coordinates.

Ground state.

4a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.176569	2.307402	0.000057
2	6	0	-1.221255	3.690753	0.000088
3	6	0	-0.050965	4.450132	0.000083
4	6	0	1.172323	3.806932	0.000054
5	6	0	1.237917	2.412997	0.000026
6	6	0	0.057270	1.639797	0.000020
7	6	0	0.279165	0.214822	-0.000023
8	6	0	1.544747	-0.311499	-0.000044
9	8	0	2.671716	0.437303	-0.000031
10	6	0	2.589241	1.806755	0.000020
11	7	0	-0.597886	-0.866820	-0.000040
12	6	0	0.115579	-2.038463	-0.000067
13	6	0	1.475677	-1.732791	-0.000063
14	6	0	-2.025813	-0.776058	-0.000029
15	6	0	-2.713461	-0.729237	-1.208311
16	6	0	-4.099314	-0.626973	-1.205037
17	6	0	-4.791927	-0.574188	-0.000004
18	6	0	-4.099312	-0.627259	1.205014
19	6	0	-2.713459	-0.729527	1.208263
20	6	0	-0.590583	-3.356354	-0.000056
21	6	0	2.649394	-2.627207	-0.000031
22	6	0	2.451258	-4.129821	0.000187
23	8	0	3.775053	-2.167293	-0.000096
24	8	0	3.615089	2.436388	-0.000040
25	1	0	-2.100925	1.746785	0.000059
26	1	0	-2.186391	4.187568	0.000115
27	1	0	-0.100734	5.533339	0.000106
28	1	0	2.106691	4.356003	0.000056
29	1	0	-2.156640	-0.764994	-2.138343
30	1	0	-4.638107	-0.587197	-2.145596
31	1	0	-5.873696	-0.492899	0.000006
32	1	0	-4.638104	-0.587704	2.145583
33	1	0	-2.156640	-0.765502	2.138287
34	1	0	-0.330828	-3.949603	-0.879975
35	1	0	-1.671201	-3.217794	-0.001044

36	1	0	-0.332351	-3.948810	0.880867
37	1	0	1.896155	-4.459654	0.882648
38	1	0	1.897097	-4.459925	-0.882774
39	1	0	3.436541	-4.594331	0.000743

4b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.755591	2.368807	-0.001964
2	6	0	0.730028	3.752594	-0.002605
3	6	0	-0.477145	4.451759	-0.001991
4	6	0	-1.666172	3.747341	-0.000887
5	6	0	-1.661115	2.351918	-0.000263
6	6	0	-0.442840	1.639342	-0.000633
7	6	0	-0.591857	0.205211	0.000222
8	6	0	-1.829203	-0.384558	0.000459
9	8	0	-2.992959	0.306278	0.000509
10	6	0	-2.979708	1.677898	0.000537
11	7	0	0.339102	-0.830224	0.000189
12	6	0	-0.314166	-2.036258	0.000317
13	6	0	-1.688314	-1.800252	0.000372
14	6	0	1.760428	-0.667195	0.000845
15	6	0	2.449406	-0.583374	1.205104
16	6	0	3.827921	-0.415531	1.199130
17	6	0	4.538960	-0.329103	0.001631
18	6	0	3.829255	-0.423829	-1.196861
19	6	0	2.451383	-0.591373	-1.203554
20	6	0	0.458102	-3.316358	0.000607
21	6	0	-2.814645	-2.753099	0.000090
22	6	0	-2.539871	-4.243666	-0.001728
23	8	0	-3.962627	-2.351783	0.001122
24	8	0	-4.036187	2.255094	0.001045
25	1	0	1.707009	1.855479	-0.002519
26	1	0	1.668702	4.297801	-0.003606
27	1	0	-0.482404	5.536101	-0.002452
28	1	0	-2.627145	4.248393	-0.000520
29	1	0	1.900524	-0.645769	2.138565
30	1	0	4.361260	-0.351645	2.142658
31	1	0	4.364002	-0.366569	-2.140131
32	1	0	1.903551	-0.659985	-2.137204
33	1	0	0.225931	-3.923515	0.878726
34	1	0	1.529996	-3.121777	0.005485

35	1	0	0.233281	-3.919716	-0.882142
36	1	0	-1.966832	-4.543408	-0.883423
37	1	0	-1.971037	-4.545879	0.881885
38	1	0	-3.500093	-4.757998	-0.004530
39	6	0	6.029339	-0.117188	-0.000178
40	1	0	6.272463	0.947503	-0.080127
41	1	0	6.486273	-0.489219	0.919317
42	1	0	6.502724	-0.623460	-0.844612

4c.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.560089	2.422058	-0.156492
2	1	0	-1.536616	1.959291	-0.204691
3	6	0	-0.456664	3.802089	-0.146424
4	1	0	-1.362177	4.399547	-0.182689
5	6	0	0.787245	4.432462	-0.092726
6	1	0	0.852952	5.514712	-0.085562
7	6	0	1.934467	3.663114	-0.051070
8	1	0	2.920390	4.111419	-0.011181
9	6	0	1.851666	2.269630	-0.059978
10	6	0	0.594853	1.626629	-0.110889
11	6	0	3.126739	1.523402	-0.017701
12	6	0	1.851803	-0.475960	-0.075481
13	6	0	0.654099	0.188026	-0.110498
14	6	0	-0.579931	-3.270812	-0.166733
15	1	0	-1.313931	-3.276782	0.644769
16	1	0	0.079730	-4.129711	-0.071441
17	1	0	-1.136693	-3.351975	-1.105417
18	6	0	0.244797	-2.029550	-0.137222
19	6	0	1.630734	-1.879526	-0.091921
20	6	0	2.623923	-2.968899	-0.063917
21	6	0	4.085252	-2.592297	-0.012470
22	1	0	4.300169	-1.986476	0.871541
23	1	0	4.359919	-1.980969	-0.875923
24	1	0	4.677034	-3.506681	0.004740
25	6	0	-1.750711	-0.571588	-0.159643
26	6	0	-2.430989	-0.368999	1.045549
27	6	0	-3.806707	-0.159106	0.982091
28	1	0	-4.349860	0.004826	1.908905
29	6	0	-4.508335	-0.152321	-0.223369
30	6	0	-3.797849	-0.359135	-1.404799

31	1	0	-4.319521	-0.353379	-2.356761
32	6	0	-2.426990	-0.569680	-1.372932
33	1	0	-1.866528	-0.723217	-2.289028
34	6	0	-6.000470	0.046342	-0.243063
35	1	0	-6.333255	0.658098	0.598446
36	1	0	-6.522610	-0.913921	-0.176441
37	1	0	-6.325644	0.531039	-1.166427
38	6	0	-1.698566	-0.351522	2.358946
39	1	0	-1.070584	-1.238126	2.480153
40	1	0	-2.400028	-0.311708	3.193863
41	1	0	-1.038907	0.518766	2.429749
42	7	0	-0.335569	-0.791460	-0.150367
43	8	0	2.289773	-4.143605	-0.080311
44	8	0	3.057104	0.149177	-0.033603
45	8	0	4.218806	2.028096	0.027716

4d.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.687699	0.206231	-0.023157
2	6	0	1.765958	-0.636292	0.058964
3	6	0	1.322316	-1.979751	0.145313
4	6	0	-0.069570	-1.912902	0.108976
5	6	0	3.346290	1.127902	-0.026342
6	6	0	2.206624	2.065898	-0.107090
7	6	0	0.860937	1.634148	-0.106416
8	6	0	-0.149782	2.604873	-0.178077
9	1	0	-1.189633	2.307676	-0.177166
10	6	0	0.176781	3.947850	-0.250412
11	1	0	-0.620703	4.682197	-0.305022
12	6	0	1.507206	4.368595	-0.253902
13	1	0	1.747948	5.424221	-0.311560
14	6	0	2.514592	3.425512	-0.181619
15	1	0	3.560856	3.708292	-0.179462
16	6	0	2.094202	-3.224995	0.254487
17	6	0	3.600713	-3.132953	0.270178
18	1	0	4.011691	-4.138626	0.350378
19	1	0	3.942269	-2.518388	1.107381
20	1	0	3.968794	-2.646014	-0.636798
21	6	0	-1.051709	-3.030787	0.184006
22	1	0	-0.939707	-3.571377	1.126725
23	1	0	-0.853900	-3.764258	-0.599928

24	1	0	-2.075751	-2.666524	0.095386
25	6	0	-1.805788	-0.141239	-0.072892
26	6	0	-2.392528	0.042362	-1.327620
27	6	0	-3.707209	0.511118	-1.367270
28	1	0	-4.181052	0.669283	-2.331514
29	6	0	-4.401527	0.779079	-0.199894
30	1	0	-5.422043	1.145014	-0.248183
31	6	0	-3.795649	0.587372	1.037474
32	1	0	-4.351267	0.805947	1.941269
33	6	0	-2.486148	0.126651	1.126317
34	6	0	-1.665621	-0.251939	-2.618668
35	1	0	-0.586198	-0.249774	-2.454389
36	1	0	-1.875157	0.558602	-3.324297
37	6	0	-2.086041	-1.584545	-3.247538
38	1	0	-1.852600	-2.425131	-2.589726
39	1	0	-1.565324	-1.744550	-4.195001
40	1	0	-3.161351	-1.605677	-3.445080
41	6	0	-1.782357	-0.076057	2.451463
42	1	0	-1.450294	-1.118317	2.516098
43	1	0	-0.860463	0.516495	2.446927
44	6	0	-2.595006	0.267916	3.694022
45	1	0	-2.899242	1.318252	3.701610
46	1	0	-1.997263	0.091326	4.590855
47	1	0	-3.496642	-0.345897	3.772422
48	7	0	-0.448329	-0.603448	0.004102
49	8	0	3.056427	-0.214977	0.059278
50	8	0	4.505961	1.450771	-0.027344
51	8	0	1.527491	-4.304909	0.330384

4e.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471958	2.366646	0.081369
2	6	0	-0.447474	3.750453	0.083436
3	6	0	0.757974	4.450833	0.032499
4	6	0	1.946487	3.747537	-0.019886
5	6	0	1.942576	2.352082	-0.022456
6	6	0	0.726059	1.638227	0.027794
7	6	0	0.876441	0.204180	0.018834
8	6	0	2.113444	-0.383983	-0.030420
9	8	0	3.275642	0.308078	-0.077482
10	6	0	3.260823	1.679436	-0.078511

11	7	0	-0.053138	-0.831921	0.055900
12	6	0	0.601324	-2.037152	0.031763
13	6	0	1.974175	-1.799944	-0.022932
14	6	0	-1.472618	-0.668238	0.109434
15	6	0	-2.208063	-0.575507	-1.062838
16	6	0	-3.587278	-0.396667	-1.020777
17	6	0	-4.232706	-0.313552	0.212927
18	6	0	-3.490410	-0.412598	1.394807
19	6	0	-2.121165	-0.589500	1.342148
20	6	0	-0.168950	-3.317896	0.063226
21	6	0	3.100544	-2.751579	-0.066268
22	6	0	2.827809	-4.242403	-0.042924
23	8	0	4.246967	-2.349381	-0.120999
24	8	0	4.315711	2.257969	-0.123284
25	1	0	-1.422024	1.852539	0.122992
26	1	0	-1.385728	4.294711	0.126331
27	1	0	0.762283	5.535189	0.034809
28	1	0	2.906211	4.249405	-0.059751
29	1	0	-1.696079	-0.634628	-2.017278
30	1	0	-4.141282	-0.324131	-1.947440
31	1	0	-4.015452	-0.346027	2.340524
32	1	0	-1.539624	-0.659582	2.255002
33	1	0	0.030428	-3.926848	-0.821718
34	1	0	-1.240245	-3.122965	0.098477
35	1	0	0.089186	-3.919308	0.938183
36	1	0	2.291941	-4.536618	0.863676
37	1	0	2.223288	-4.551173	-0.900178
38	1	0	3.787922	-4.755879	-0.076472
39	8	0	-5.565181	-0.140044	0.371048
40	6	0	-6.371456	-0.026862	-0.784789
41	1	0	-7.392176	0.107476	-0.429027
42	1	0	-6.084476	0.839147	-1.391780
43	1	0	-6.320797	-0.931919	-1.400516

4f.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.456577	2.382295	-0.000378
2	6	0	-0.417332	3.765949	-0.000482
3	6	0	0.796951	4.452188	-0.000352
4	6	0	1.978733	3.735419	-0.000136
5	6	0	1.959399	2.340244	-0.000035

6	6	0	0.733824	1.640361	-0.000136
7	6	0	0.869058	0.204470	-0.000001
8	6	0	2.099986	-0.397909	0.000115
9	8	0	3.270268	0.280499	0.000178
10	6	0	3.271232	1.652881	0.000141
11	7	0	-0.071854	-0.823075	-0.000086
12	6	0	0.570454	-2.036836	-0.000031
13	6	0	1.945418	-1.812626	0.000068
14	6	0	-1.489645	-0.647786	-0.000011
15	6	0	-2.176878	-0.560835	-1.206169
16	6	0	-3.553189	-0.378902	-1.210457
17	6	0	-4.229397	-0.287888	0.000134
18	6	0	-3.552934	-0.377935	1.210657
19	6	0	-2.176626	-0.559876	1.206226
20	6	0	-0.213094	-3.310224	-0.000071
21	6	0	3.064279	-2.776049	0.000082
22	6	0	2.776999	-4.263853	-0.000527
23	8	0	4.214646	-2.382873	0.000628
24	8	0	4.333302	2.218738	0.000257
25	1	0	-1.414289	1.880846	-0.000494
26	1	0	-1.350446	4.320430	-0.000669
27	1	0	0.813487	5.536354	-0.000429
28	1	0	2.944727	4.226700	-0.000049
29	1	0	-1.627952	-0.628417	-2.138842
30	1	0	-4.099423	-0.307208	-2.143252
31	1	0	-4.098973	-0.305503	2.143510
32	1	0	-1.627502	-0.626731	2.138835
33	1	0	0.009356	-3.916794	-0.881091
34	1	0	-1.283839	-3.108998	0.001244
35	1	0	0.011308	-3.917988	0.879598
36	1	0	2.204261	-4.560406	0.882470
37	1	0	2.203218	-4.559626	-0.883095
38	1	0	3.732765	-4.786352	-0.001256
39	17	0	-5.956673	-0.058484	0.000224

Excited State:

4a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.290564	2.241758	-0.000013
2	6	0	-1.426476	3.634915	0.000122
3	6	0	-0.263722	4.428414	0.000162

4	6	0	1.000158	3.867153	0.000045
5	6	0	1.171775	2.460464	-0.000138
6	6	0	-0.034385	1.641652	-0.000121
7	6	0	0.263226	0.251126	-0.000173
8	6	0	1.598396	-0.250725	-0.000130
9	8	0	2.682327	0.491608	-0.000134
10	6	0	2.502640	1.953546	-0.000290
11	7	0	-0.558279	-0.859096	-0.000170
12	6	0	0.204304	-2.012880	-0.000140
13	6	0	1.555392	-1.667582	-0.000086
14	6	0	-1.991596	-0.837306	-0.000071
15	6	0	-2.677397	-0.827337	-1.209495
16	6	0	-4.066507	-0.798523	-1.205367
17	6	0	-4.760020	-0.782215	0.000133
18	6	0	-4.066330	-0.798540	1.205528
19	6	0	-2.677219	-0.827362	1.209452
20	6	0	-0.456658	-3.347539	-0.000025
21	6	0	2.757872	-2.533453	0.000078
22	6	0	2.601761	-4.040296	0.000190
23	8	0	3.866111	-2.039090	0.000122
24	8	0	3.546588	2.561308	0.000227
25	1	0	-2.181235	1.628902	-0.000005
26	1	0	-2.409370	4.088150	0.000216
27	1	0	-0.357523	5.510349	0.000271
28	1	0	1.887480	4.487848	0.000046
29	1	0	-2.120522	-0.829414	-2.140126
30	1	0	-4.606797	-0.785299	-2.145613
31	1	0	-5.844429	-0.756643	0.000213
32	1	0	-4.606481	-0.785326	2.145854
33	1	0	-2.120212	-0.829454	2.140003
34	1	0	-0.167986	-3.930526	-0.878442
35	1	0	-1.540858	-3.248776	-0.001638
36	1	0	-0.170548	-3.929127	0.880202
37	1	0	2.058179	-4.387056	0.883344
38	1	0	2.059741	-4.387193	-0.883882
39	1	0	3.600406	-4.474990	0.001051

4b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.794562	2.351391	-0.004556
2	6	0	0.812215	3.751417	-0.004131

3	6	0	-0.413205	4.443788	-0.000947
4	6	0	-1.625109	3.777671	0.001152
5	6	0	-1.677113	2.361411	0.000002
6	6	0	-0.406308	1.647439	-0.002290
7	6	0	-0.585308	0.236488	-0.001251
8	6	0	-1.873644	-0.375870	-0.000728
9	8	0	-3.016468	0.272401	-0.001324
10	6	0	-2.960477	1.744037	0.000935
11	7	0	0.326956	-0.800039	-0.000436
12	6	0	-0.335809	-2.013645	0.000312
13	6	0	-1.711463	-1.783932	0.000058
14	6	0	1.753125	-0.657734	0.000591
15	6	0	2.439919	-0.588353	1.206355
16	6	0	3.821154	-0.447662	1.200067
17	6	0	4.533535	-0.374526	0.002266
18	6	0	3.823082	-0.455602	-1.196933
19	6	0	2.442448	-0.596111	-1.204829
20	6	0	0.435566	-3.287442	0.001153
21	6	0	-2.836337	-2.748046	0.000185
22	6	0	-2.553638	-4.236519	-0.001371
23	8	0	-3.982589	-2.349414	0.001431
24	8	0	-4.051880	2.262005	0.003238
25	1	0	1.733748	1.815785	-0.006663
26	1	0	1.753271	4.286197	-0.005962
27	1	0	-0.411281	5.529808	-0.000160
28	1	0	-2.561746	4.321082	0.003511
29	1	0	1.890171	-0.635884	2.140154
30	1	0	4.355181	-0.392293	2.143538
31	1	0	4.358968	-0.406602	-2.139807
32	1	0	1.894235	-0.649712	-2.139212
33	1	0	0.194159	-3.893919	0.877885
34	1	0	1.507248	-3.095905	0.006848
35	1	0	0.202971	-3.889882	-0.880881
36	1	0	-1.980982	-4.535369	-0.883645
37	1	0	-1.986008	-4.537619	0.883433
38	1	0	-3.512176	-4.753717	-0.004502
39	6	0	6.027039	-0.188735	0.001084
40	1	0	6.286444	0.872492	-0.071841
41	1	0	6.477903	-0.574032	0.918027
42	1	0	6.491289	-0.696871	-0.847180

4c.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.613129	2.393701	-0.283343
2	1	0	-1.569675	1.901190	-0.398351
3	6	0	-0.564171	3.793304	-0.237471
4	1	0	-1.473244	4.375258	-0.317283
5	6	0	0.683736	4.419936	-0.077304
6	1	0	0.732775	5.503593	-0.025973
7	6	0	1.858824	3.693510	0.014576
8	1	0	2.813587	4.189884	0.135829
9	6	0	1.846425	2.279204	-0.057938
10	6	0	0.547195	1.632805	-0.187614
11	6	0	3.096435	1.599098	-0.002164
12	6	0	1.899354	-0.464449	-0.128041
13	6	0	0.648266	0.213925	-0.170899
14	6	0	-0.535344	-3.252511	-0.111285
15	1	0	-1.283471	-3.220403	0.687085
16	1	0	0.122995	-4.107219	0.020204
17	1	0	-1.084824	-3.361464	-1.052851
18	6	0	0.278664	-2.012956	-0.121794
19	6	0	1.668384	-1.854599	-0.096952
20	6	0	2.666329	-2.946736	-0.047006
21	6	0	4.125001	-2.570864	-0.027671
22	1	0	4.349386	-1.927671	0.826888
23	1	0	4.386891	-1.990994	-0.916408
24	1	0	4.716500	-3.484374	0.017237
25	6	0	-1.740807	-0.580454	-0.158375
26	6	0	-2.402490	-0.345536	1.050679
27	6	0	-3.783315	-0.171119	1.001354
28	1	0	-4.314933	0.019578	1.929515
29	6	0	-4.503897	-0.228058	-0.191770
30	6	0	-3.808553	-0.465039	-1.376598
31	1	0	-4.345299	-0.506898	-2.318998
32	6	0	-2.432921	-0.642626	-1.360490
33	1	0	-1.884423	-0.814843	-2.280587
34	6	0	-5.999859	-0.061820	-0.193163
35	1	0	-6.327893	0.605158	0.607174
36	1	0	-6.498868	-1.024778	-0.042077
37	1	0	-6.354234	0.344981	-1.142749
38	6	0	-1.648756	-0.250530	2.348372
39	1	0	-1.004339	-1.119765	2.507339
40	1	0	-2.337128	-0.180197	3.191822
41	1	0	-1.006299	0.635192	2.361087
42	7	0	-0.318576	-0.773505	-0.164644

43	8	0	2.319387	-4.116275	-0.021181
44	8	0	3.081296	0.127974	-0.127664
45	8	0	4.209357	2.051950	0.130469

4d.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.683103	0.242174	-0.012898
2	6	0	1.816232	-0.615846	0.072815
3	6	0	1.374406	-1.947318	0.149509
4	6	0	-0.024218	-1.897084	0.108219
5	6	0	3.324829	1.230845	-0.034882
6	6	0	2.192992	2.092956	-0.110932
7	6	0	0.801185	1.656872	-0.092391
8	6	0	-0.229961	2.589414	-0.155959
9	1	0	-1.258419	2.254561	-0.140845
10	6	0	0.040559	3.961403	-0.243400
11	1	0	-0.770571	4.676380	-0.291376
12	6	0	1.380571	4.384781	-0.272231
13	1	0	1.602730	5.445281	-0.345125
14	6	0	2.431479	3.485096	-0.209679
15	1	0	3.459237	3.825449	-0.231884
16	6	0	2.159971	-3.190784	0.257106
17	6	0	3.662097	-3.086597	0.282041
18	1	0	4.080894	-4.089268	0.357802
19	1	0	3.992142	-2.471675	1.123427
20	1	0	4.029839	-2.586617	-0.617760
21	6	0	-0.984548	-3.024514	0.175717
22	1	0	-0.840386	-3.580090	1.106126
23	1	0	-0.773393	-3.744109	-0.618995
24	1	0	-2.015581	-2.679806	0.104748
25	6	0	-1.800618	-0.164618	-0.072619
26	6	0	-2.394538	-0.009619	-1.327014
27	6	0	-3.727561	0.404090	-1.362194
28	1	0	-4.210628	0.541431	-2.324837
29	6	0	-4.427633	0.647554	-0.193008
30	1	0	-5.462311	0.971214	-0.239123
31	6	0	-3.809640	0.489869	1.043237
32	1	0	-4.369178	0.693293	1.947981
33	6	0	-2.482121	0.084789	1.129367
34	6	0	-1.659894	-0.267525	-2.621437
35	1	0	-0.580422	-0.228186	-2.462315

36	1	0	-1.896336	0.544702	-3.315954
37	6	0	-2.037394	-1.604722	-3.267586
38	1	0	-1.777955	-2.447978	-2.622601
39	1	0	-1.512459	-1.734722	-4.217096
40	1	0	-3.111389	-1.657904	-3.465472
41	6	0	-1.758979	-0.064783	2.451077
42	1	0	-1.354629	-1.081310	2.520869
43	1	0	-0.883470	0.594859	2.437721
44	6	0	-2.586431	0.228310	3.696803
45	1	0	-2.953070	1.258218	3.705555
46	1	0	-1.974882	0.089350	4.590778
47	1	0	-3.448447	-0.439609	3.778384
48	7	0	-0.427225	-0.588030	0.003766
49	8	0	3.076953	-0.215949	0.084385
50	8	0	4.500884	1.512071	-0.050634
51	8	0	1.591656	-4.269336	0.323208

4e.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470669	2.374372	0.181399
2	6	0	-0.437559	3.757363	0.215899
3	6	0	0.769707	4.452145	0.134875
4	6	0	1.951249	3.743695	0.024486
5	6	0	1.939645	2.348475	-0.009396
6	6	0	0.719280	1.640365	0.063581
7	6	0	0.852725	0.206005	0.015838
8	6	0	2.087352	-0.380349	-0.057875
9	8	0	3.259264	0.301908	-0.117974
10	6	0	3.254359	1.673420	-0.112853
11	7	0	-0.074086	-0.825385	0.069503
12	6	0	0.584741	-2.041179	0.022546
13	6	0	1.965290	-1.800326	-0.038838
14	6	0	-1.492296	-0.676023	0.106857
15	6	0	-2.202127	-0.446248	-1.063395
16	6	0	-3.583719	-0.282434	-1.034890
17	6	0	-4.260148	-0.359665	0.182213
18	6	0	-3.546352	-0.600643	1.360731
19	6	0	-2.173996	-0.757276	1.321660
20	6	0	-0.169507	-3.327335	0.006498
21	6	0	3.059582	-2.708821	-0.066699

22	6	0	3.025762	-4.199517	0.134722
23	8	0	4.272948	-2.272711	-0.312815
24	8	0	4.311260	2.246150	-0.185642
25	1	0	-1.420435	1.861968	0.249142
26	1	0	-1.369840	4.305688	0.308833
27	1	0	0.781151	5.536121	0.161618
28	1	0	2.911760	4.242072	-0.035785
29	1	0	-1.666286	-0.385513	-2.004544
30	1	0	-4.115380	-0.098934	-1.959354
31	1	0	-4.095233	-0.656166	2.293603
32	1	0	-1.614099	-0.934223	2.233589
33	1	0	0.289272	-4.035372	-0.687041
34	1	0	-1.199918	-3.168684	-0.315511
35	1	0	-0.209629	-3.807866	0.991752
36	1	0	2.097720	-4.492380	0.622288
37	1	0	3.123404	-4.745269	-0.812536
38	1	0	3.862371	-4.504410	0.771863
39	8	0	-5.599004	-0.216723	0.326543
40	6	0	-6.376605	0.033103	-0.826906
41	1	0	-7.407468	0.115472	-0.484541
42	1	0	-6.083225	0.969498	-1.314787
43	1	0	-6.301606	-0.788056	-1.548743

4f.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265068	1.712838	-0.001356
2	6	0	-1.724801	3.019256	-0.002054
3	6	0	-0.838130	4.091953	-0.001735
4	6	0	0.535173	3.863821	-0.000833
5	6	0	1.020085	2.566914	-0.000173
6	6	0	0.122179	1.463511	-0.000306
7	6	0	0.743015	0.187117	0.000516
8	6	0	2.175584	0.068280	0.000568
9	8	0	2.998586	1.111913	0.000634
10	6	0	2.491175	2.406527	0.000519
11	7	0	0.237999	-1.080965	0.000730
12	6	0	1.278756	-1.966976	0.000553
13	6	0	2.522172	-1.273012	0.000260
14	6	0	-1.166107	-1.471123	0.001395
15	6	0	-1.889959	-1.304962	-1.237147

16	6	0	-3.238193	-1.065236	-1.223843
17	6	0	-3.929318	-0.921089	0.000354
18	6	0	-3.238306	-1.060733	1.224999
19	6	0	-1.890005	-1.300374	1.239325
20	6	0	1.009816	-3.421197	0.000886
21	6	0	3.919059	-1.775808	-0.000385
22	6	0	4.186483	-3.261885	-0.002834
23	8	0	4.835683	-0.979906	0.001044
24	8	0	3.282246	3.303536	0.000863
25	1	0	-1.965501	0.894761	-0.001675
26	1	0	-2.793764	3.198021	-0.002862
27	1	0	-1.213719	5.109067	-0.002255
28	1	0	1.245160	4.682137	-0.000669
29	1	0	-1.372992	-1.422570	-2.184648
30	1	0	-3.789702	-0.997923	-2.155684
31	1	0	-3.789882	-0.990029	2.156556
32	1	0	-1.373141	-1.414747	2.187268
33	1	0	1.445757	-3.895774	-0.882430
34	1	0	-0.069186	-3.571076	0.005971
35	1	0	1.455361	-3.897371	0.878414
36	1	0	3.760046	-3.743963	0.880890
37	1	0	3.753917	-3.742650	-0.884248
38	1	0	5.265894	-3.406196	-0.006438
39	17	0	-5.652824	-0.592130	-0.000345
