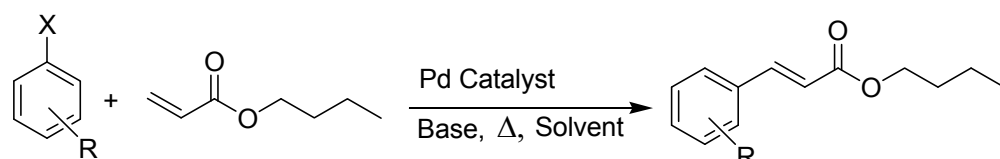


Supporting Information

Contents

| | |
|---|-----|
| Table S1. Heck coupling reactions of aryl halides and <i>n</i> -butylacrylate with different bases | S2 |
| Table S2. Heck coupling reactions of aryl halide and styrene with different bases | S2 |
| Experimental | S3 |
| Figure S1. ¹ H-NMR of 3-phenylacrylic acid <i>n</i> -butyl ester | S4 |
| Figure S2. ¹ H-NMR of 3-(4-nitrophenyl)acrylic acid <i>n</i> -butyl ester | S5 |
| Figure S3. ¹ H-NMR of 3-(4-cyanophenyl)acrylic acid <i>n</i> -butyl ester | S6 |
| Figure S4. ¹ H-NMR of 3-(4-methoxyphenyl)acrylic acid <i>n</i> -butyl ester | S7 |
| Figure S5. ¹ H-NMR of stilbene | S8 |
| Figure S6. ¹ H NMR of 4-methoxystilbene | S9 |
| Figure S7. ¹ H NMR of 4-cyanostilbene | S10 |
| Figure S8. GC-MS data of 3-phenylacrylic acid <i>n</i> -butyl ester | S11 |
| Figure S9. GC-MS data of 3-(4-methoxyphenyl)acrylic acid <i>n</i> -butyl ester | S12 |
| Figure S10. GC-MS data of 3-(4-cyanophenyl)acrylic acid <i>n</i> -butyl ester | S13 |
| Figure S11. GC-MS data of 3-(4-nitrophenyl)acrylic acid <i>n</i> -butyl ester | S14 |
| Figure S12. GC-MS data of 4-methoxystilbene | S15 |
| Figure S13. GC-MS data of stilbene | S16 |
| Figure S14. GC-MS data of 4-cyanostilbene | S17 |

Table S1. Heck coupling reaction of aryl halides with *n*-butylacrylate with different solvents and bases using 0.005 mol % catalyst.

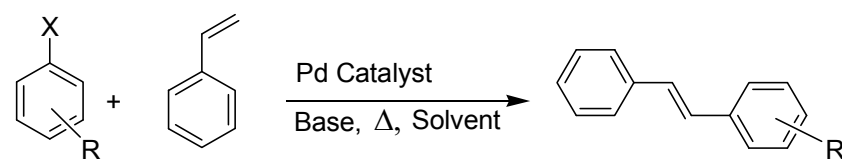


| Entry | X | R | Solvent | Base | Time/h | Temp/°C | Yield(%) ^b |
|-------|----------------|---------------|------------------------|---------------------------------|--------|---------|-----------------------|
| 1 | I | H | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 2 | Br | H | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 3 | Br | <i>m</i> -MeO | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 4 | Br | <i>o</i> -MeO | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 5 | Br | <i>m</i> -Me | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 6 | Br | <i>m</i> -Cl | DMF | Cs ₂ CO ₃ | 20 | 140 | 0 |
| 7 | I | H | DMF/H ₂ O * | Cs ₂ CO ₃ | 5 | 145 | 0 |
| 8 | I | H | MeOH | LiOH·H ₂ O | 5 | 65 | 0 |
| 9 | Br | H | DMF | Cy ₂ NMe | 15 | 140 | 0 |
| 10 | Br | H | NMP ⁺ | Cs ₂ CO ₃ | 12 | 100 | 0 |
| 11 | I | H | DMF/H ₂ O * | Cs ₂ CO ₃ | 14 | 145 | 0 |
| 12 | I | H | DMF | Cy ₂ NMe | 5 | 145 | 0 |
| 13 | I ^a | H | DMF | NBu ₃ | 5 | 140 | 96 |

^a reaction with 0.05 mol % catalyst; ^b GC-MS yield; * Solvent mixture was in 4 (DMF):1 (H₂O) ratio;

⁺ *N*-Methyl-2-pyrrolidone.

Table S2. Heck coupling reaction of aryl halides with styrene with different bases using 0.005 mol % catalyst.



| Entry | X | R | DMF/H ₂ O (v/v) | Base | Time/h | Temp/°C | Yield(%) ^c |
|-------|-----------------|---------------------------|----------------------------|---------------------------------|--------|---------|-----------------------|
| 1 | I | H | DMF | Cs ₂ CO ₃ | 20 | 140 | 33 |
| 2 | I | H | 4:1 | Cs ₂ CO ₃ | 4 | 140 | 51 |
| 3 | Br | H | 4:1 | Cs ₂ CO ₃ | 4 | 140 | 0 |
| 4 | Br | <i>m</i> -Cl | 4:1 | Cs ₂ CO ₃ | 4 | 140 | 0 |
| 5 | Br | <i>m</i> -MeO | 4:1 | Cs ₂ CO ₃ | 4 | 140 | 0 |
| 6 | Br | H | 4:1 | Cs ₂ CO ₃ | 12 | 80 | 0 |
| 7 | Br | <i>m</i> -MeO | DMF | K ₂ CO ₃ | 12 | 70 | 0 |
| 8 | Br | H | DMF | NaOAc | 12 | 100 | 0 |
| 9 | Br ^a | H | 4:1 | Cs ₂ CO ₃ | 14 | 140 | 0 |
| 10 | Br | H | 4:1 | Cy ₂ NMe | 15 | 140 | 0 |
| 11 | I | <i>p</i> -NO ₂ | 7:1 | Cs ₂ CO ₃ | 4 | 150 | 0 |
| 12 | I | <i>p</i> -MeO | 4:1 | Cs ₂ CO ₃ | 4 | 150 | 0 |
| 13 | I ^b | H | DMF | NBu ₃ | 5 | 140 | 55 |

^a reaction with 0.05 mol % catalyst; ^b reaction with 0.01 mol % catalyst; ^c GC-MS yield.

Experimental

3-Phenylacrylic acid n-butyl ester (1a). Yellow oil. $^1\text{H-NMR}$: δ 0.97 (t, $J = 7.4$ Hz, 3H), 1.40–1.49 (m, 2H), 1.66–1.73 (m, 2H), 4.21 (t, $J = 6.8$ Hz, 2H), 6.44 (d, $J = 8.0$ Hz, 1H), 7.37–7.39 (m, 3H), 7.51–7.54 (m, 2H), 7.68 (d, $J = 16.4$ Hz, 1H)

3-(4-Nitrophenyl)acrylic acid n-butyl ester (1b). Yellow solid. $^1\text{H-NMR}$: δ 0.97 (t, $J = 7.4$ Hz, 3H), 1.40–1.49 (m, 2H), 1.67–1.74 (m, 2H), 4.24 (t, $J = 6.8$ Hz, 2H), 6.56 (d, $J = 16.0$ Hz, 1H), 7.66–7.72 (m, 3H), 8.25 (d, $J = 9.2$ Hz, 2H)

3-(4-Cyanophenyl)acrylic acid n-butyl ester (1c). Yellow oil. $^1\text{H-NMR}$: δ 0.96 (t, $J = 7.4$ Hz, 3H), 1.39–1.48 (m, 2H), 1.66–1.71 (m, 2H), 4.23 (t, $J = 6.8$ Hz, 2H), 6.52 (d, $J = 16$ Hz, 1H), 7.60–7.69 (m, 5H)

3-(4-Methoxyphenyl)acrylic acid n-butyl ester (1d). Yellow oil. $^1\text{H-NMR}$: δ 0.96 (t, $J = 7.4$ Hz, 3H), 1.39–1.48 (m, 2H), 1.65–1.72 (m, 2H), 3.84 (s, 3H), 4.20 (t, $J = 6.7$ Hz, 2H), 6.31 (d, $J = 16.0$ Hz, 1H), 6.90 (d, $J = 8.8$ Hz, 2H), 7.48 (d, $J = 8.6$ Hz, 2H), 7.64 (d, $J = 16.0$ Hz, 1H)

Stilbene (1e). Colorless solid. $^1\text{H-NMR}$: δ 7.12 (s, 2H), 7.29 (t, $J = 6.6$ Hz, 2H), 7.36 (t, $J = 7.6$ Hz, 4H), 7.52 (dd, $J = 8.2$ Hz, 4H)

4-Methoxystilbene (1f). Colorless solid. $^1\text{H-NMR}$: δ 3.83 (s, 3H), 6.90 (d, $J = 8.8$ Hz, 2H), 6.98 (d, $J = 16.3$ Hz, 1H), 7.07 (d, $J = 16.3$ Hz, 1H), 7.21–7.25 (m, 1H), 7.35 (t, $J = 7.6$ Hz, 2H), 7.44–7.50 (m, 4H)

4-Cyanostilbene (1g). Colorless solid. $^1\text{H-NMR}$: δ 7.09 (d, $J = 16.3$ Hz, 1H), 7.22 (d, $J = 16.3$ Hz, 1H), 7.30–7.34 (m, 1H), 7.39 (t, $J = 7.5$ Hz, 1H), 7.52–7.65 (m, 6H)

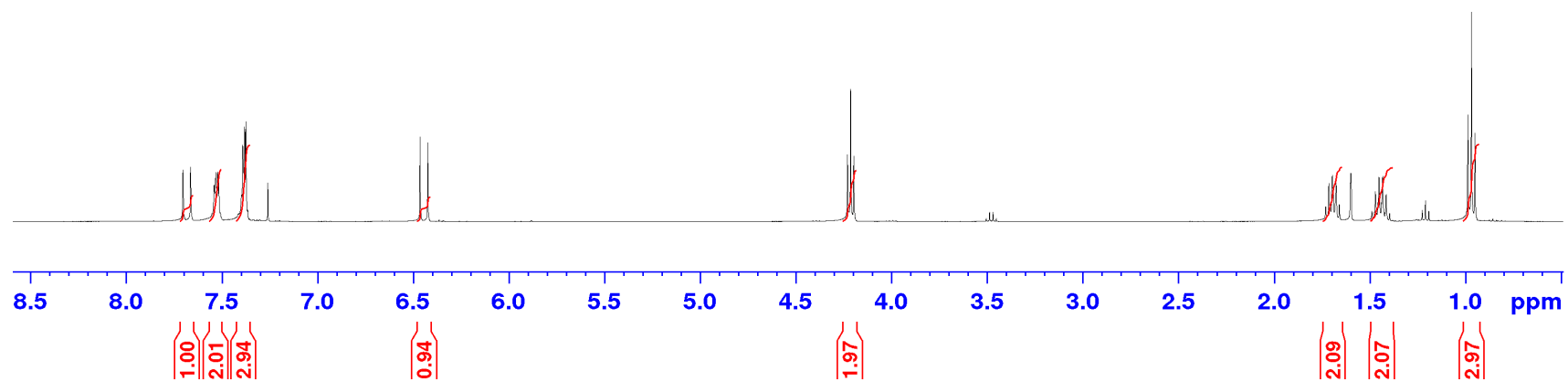
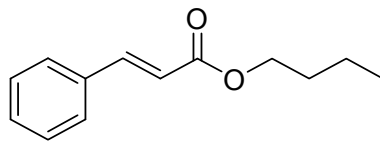


Figure S1. ¹H-NMR of 3-phenylacrylic acid *n*-butyl ester.

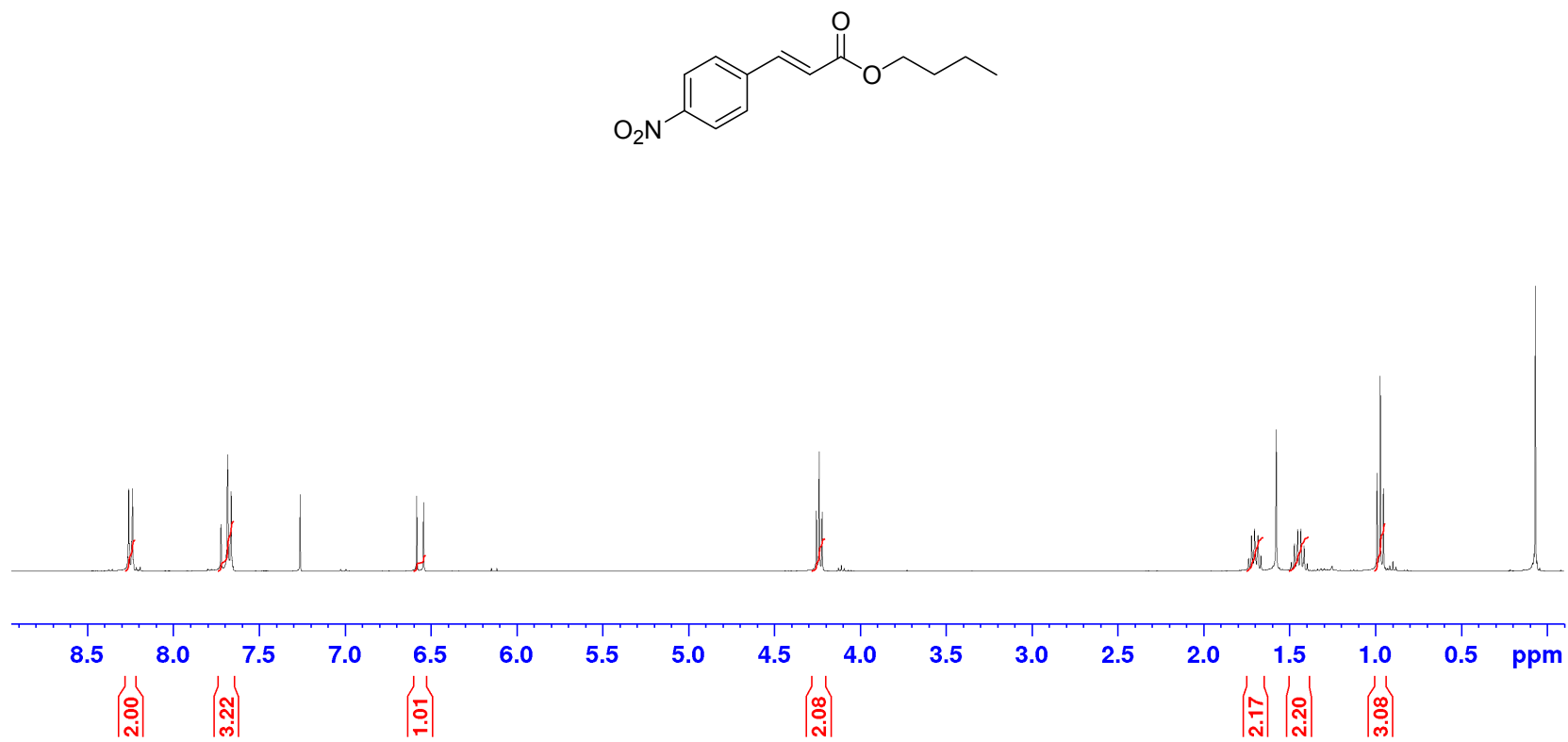


Figure S2. ¹H-NMR of 3-(4-nitrophenyl)acrylic acid *n*-butyl ester.

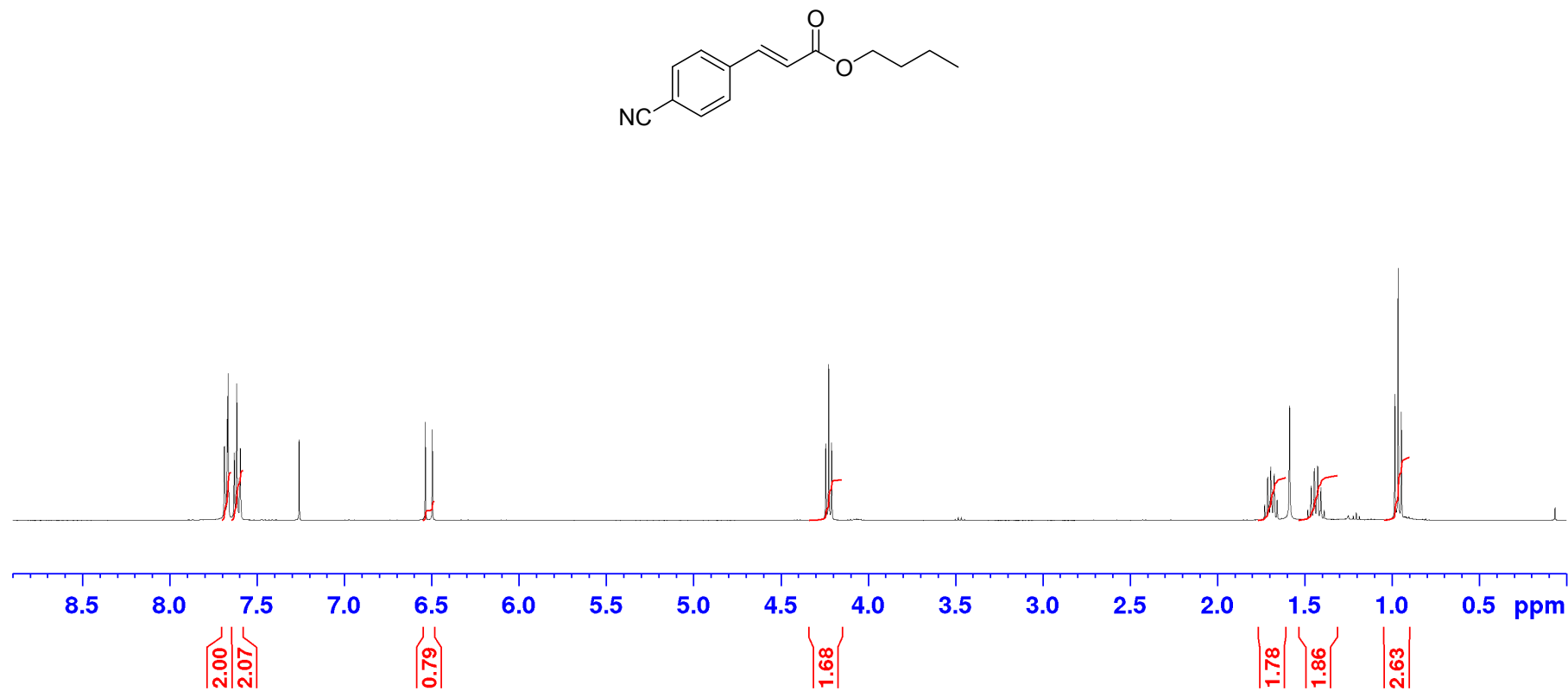


Figure S3. ¹H-NMR of 3-(4-cyanophenyl)acrylic acid *n*-butyl ester.

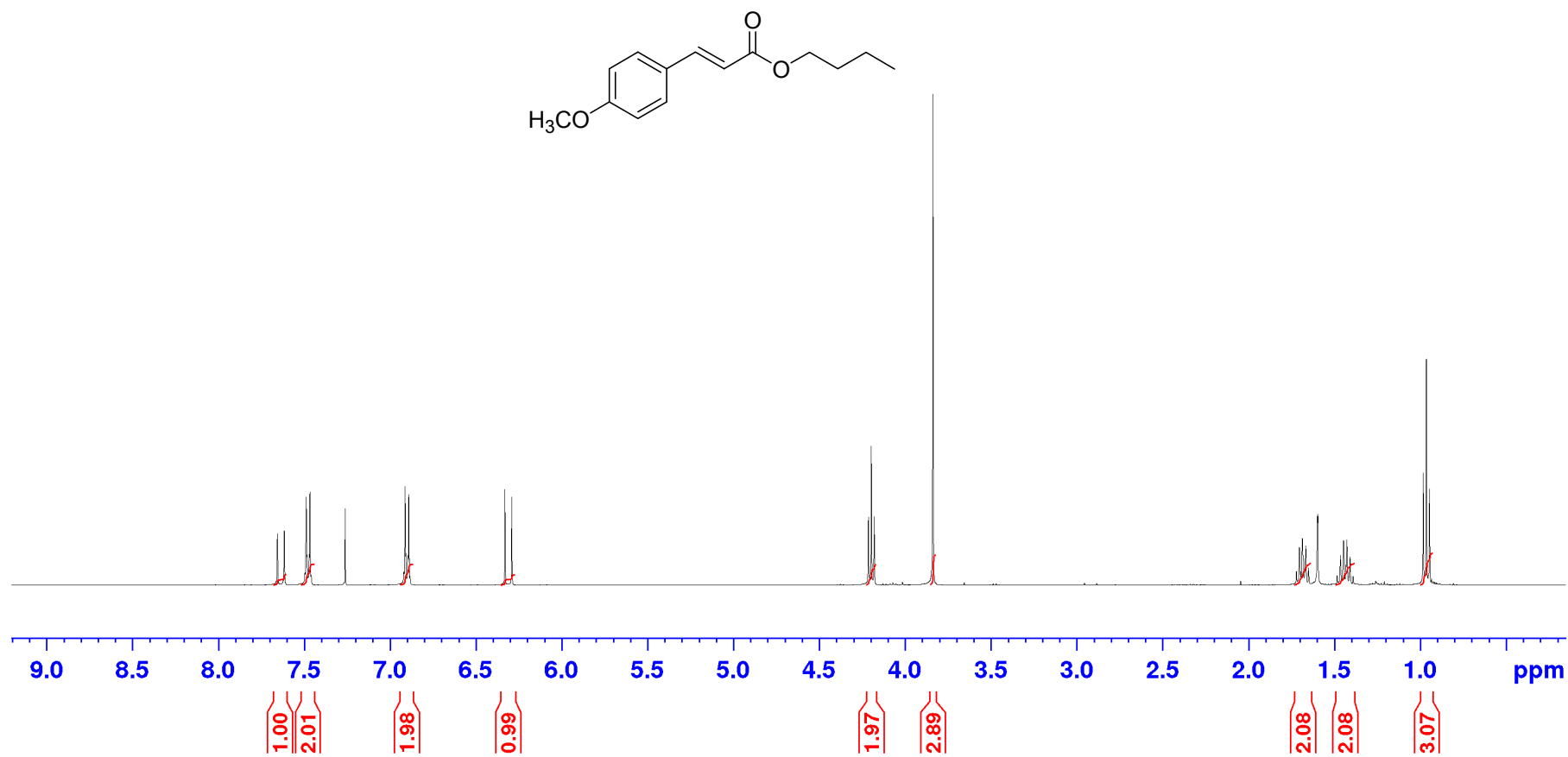


Figure S4. ¹H-NMR of 3-(4-methoxyphenyl)acrylic acid *n*-butyl ester.

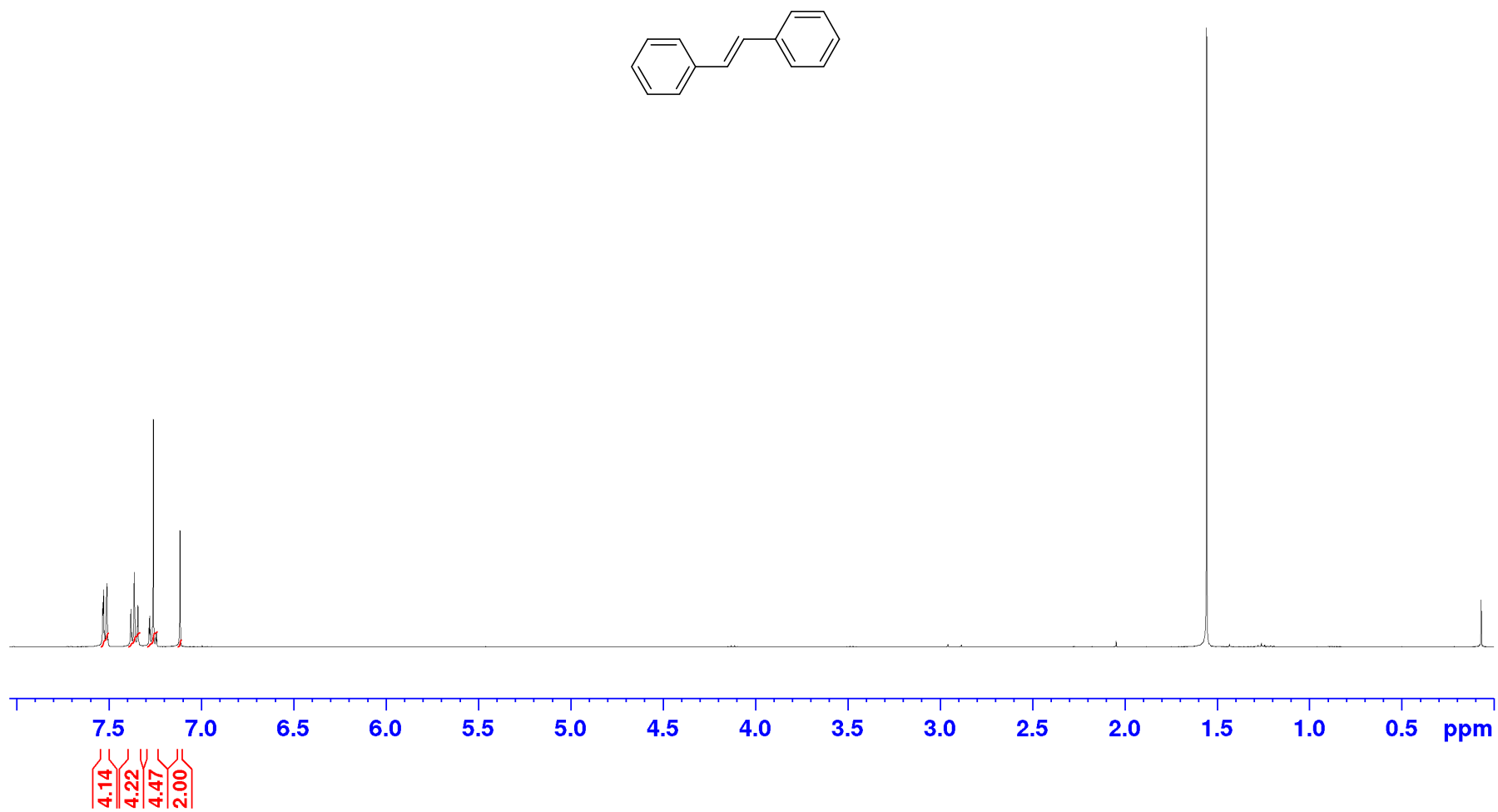


Figure S5. ¹H-NMR of stilbene.

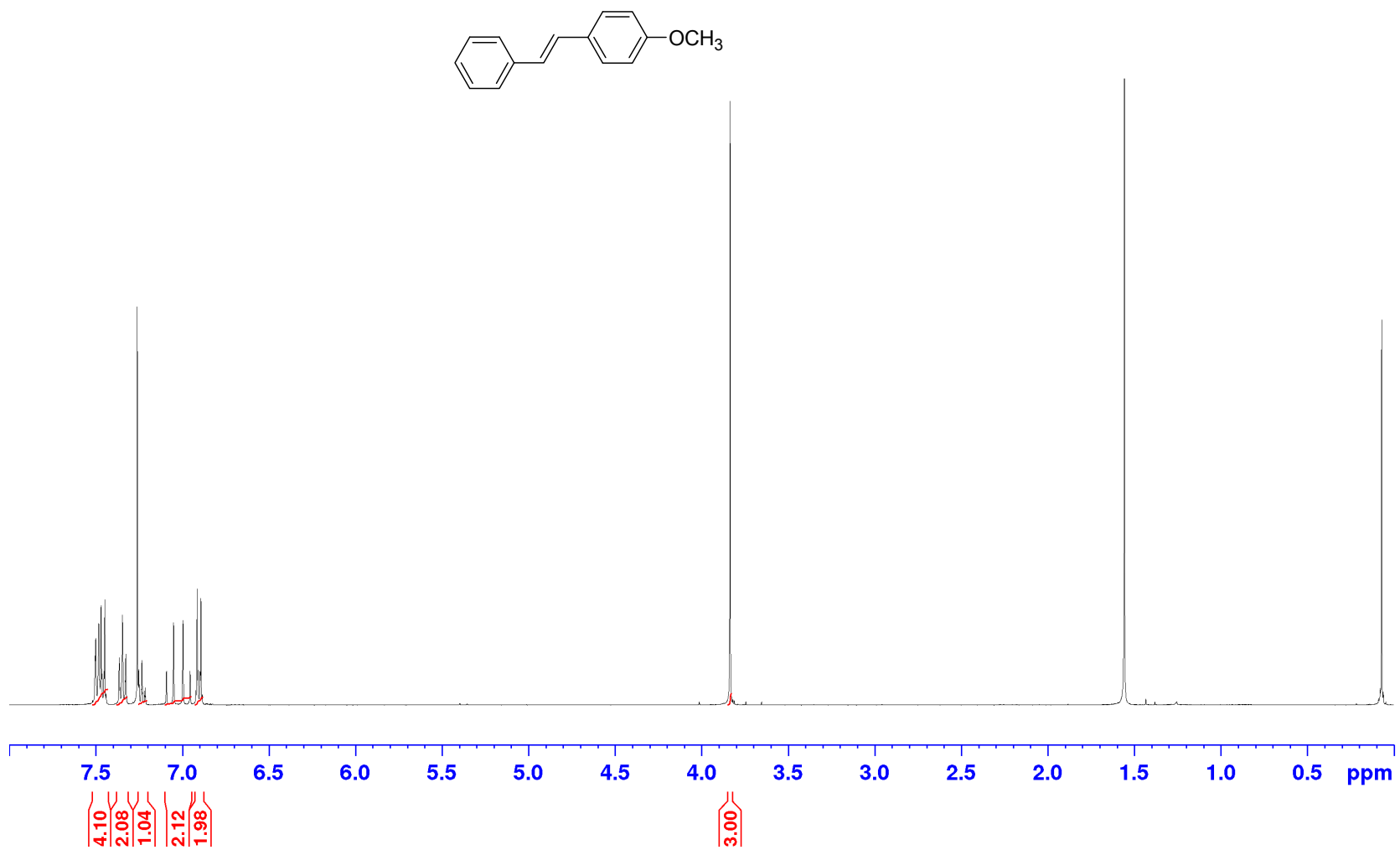


Figure S6. ¹H-NMR of 4-methoxystilbene.

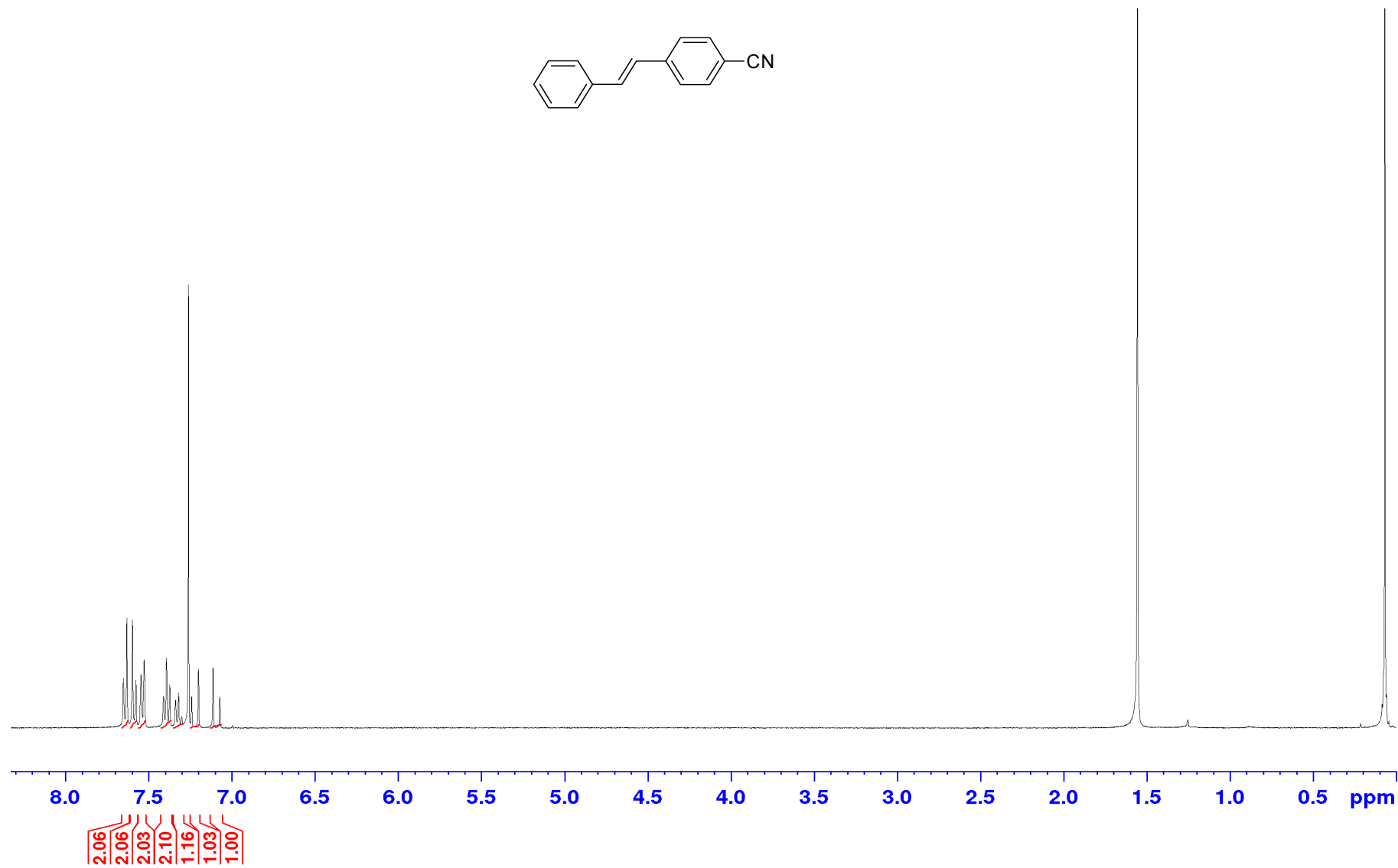


Figure S7. ¹H-NMR of 4-cyanostilbene.

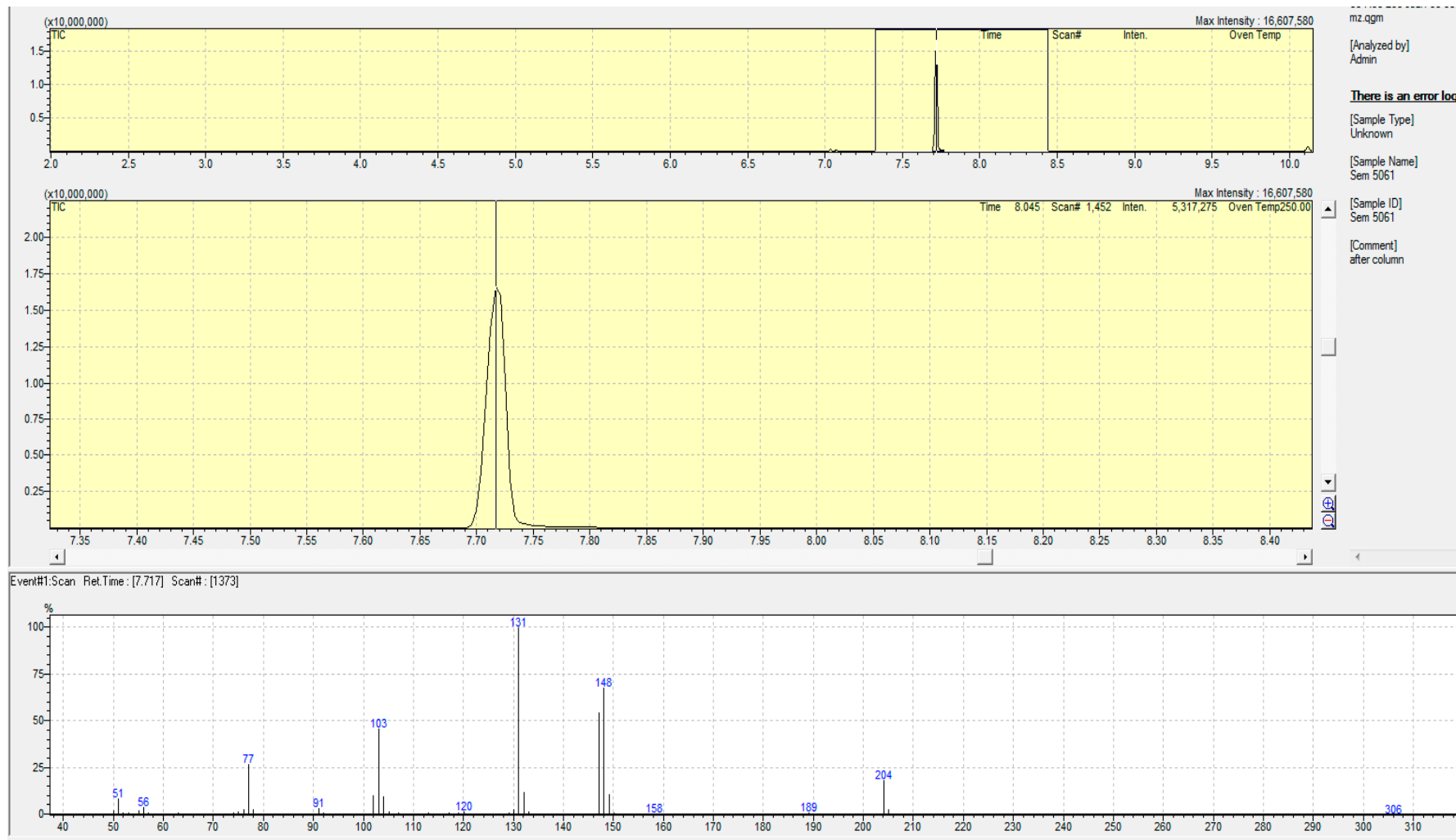


Figure S1. GC-MS data of 3-phenylacrylic acid *n*-butyl ester. $m/z = 204$.

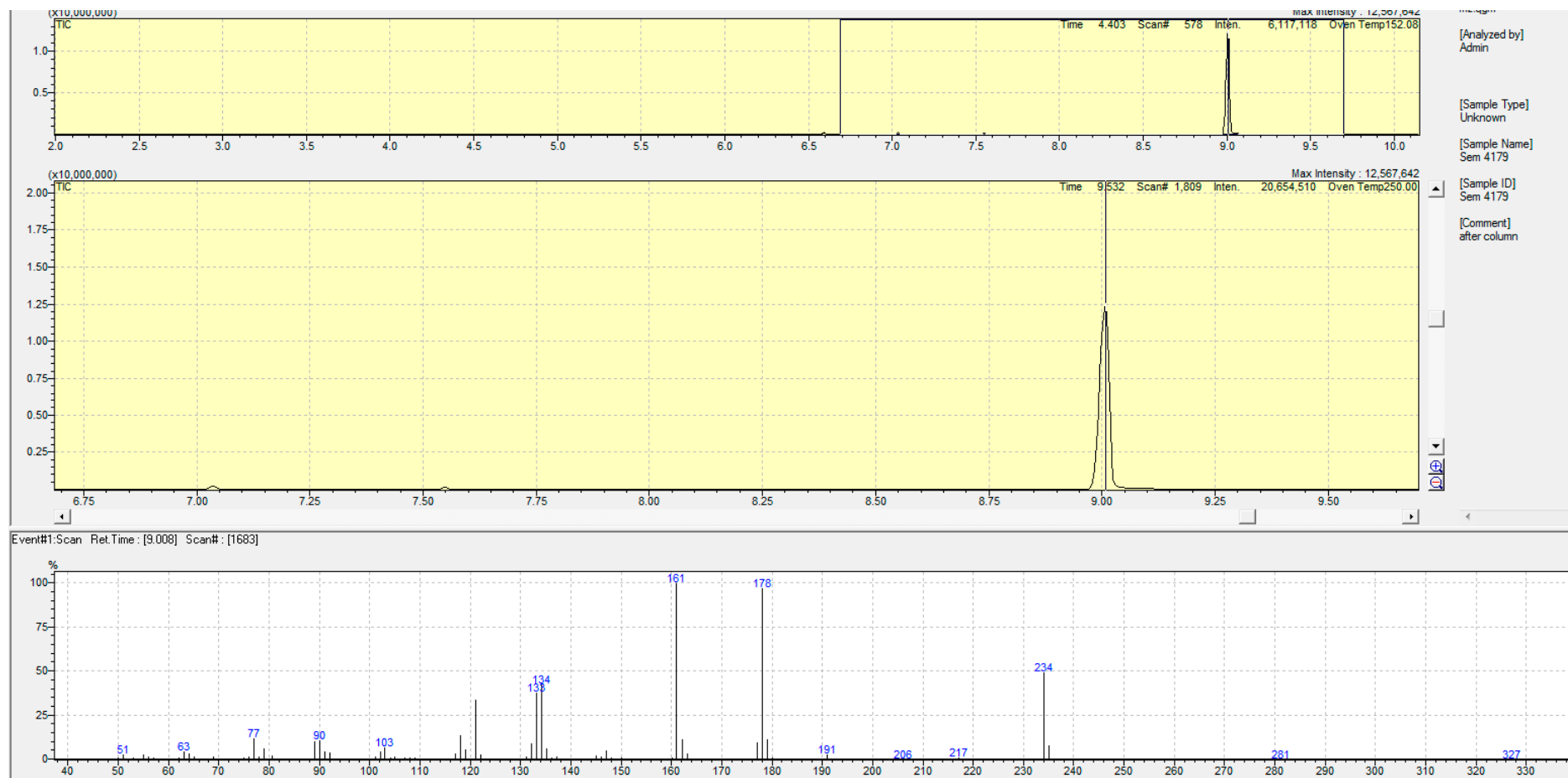


Figure S9. GC-MS data of 3-(4-methoxyphenyl)acrylic acid *n*-butyl ester. $m/z = 234$.

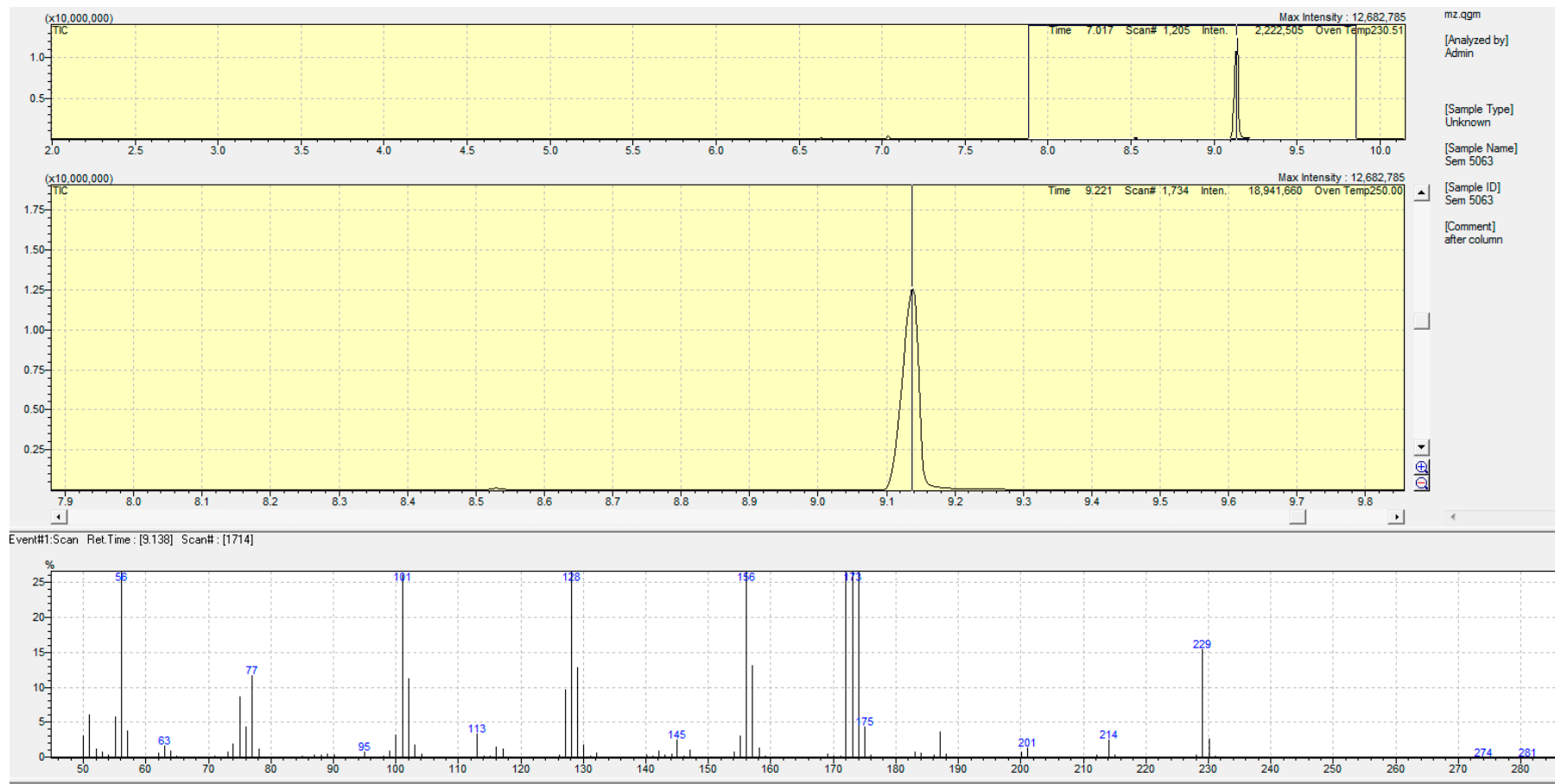


Figure S10. GC-MS data of 3-(4-cyanophenyl)acrylic acid *n*-butyl ester. $m/z = 229$.

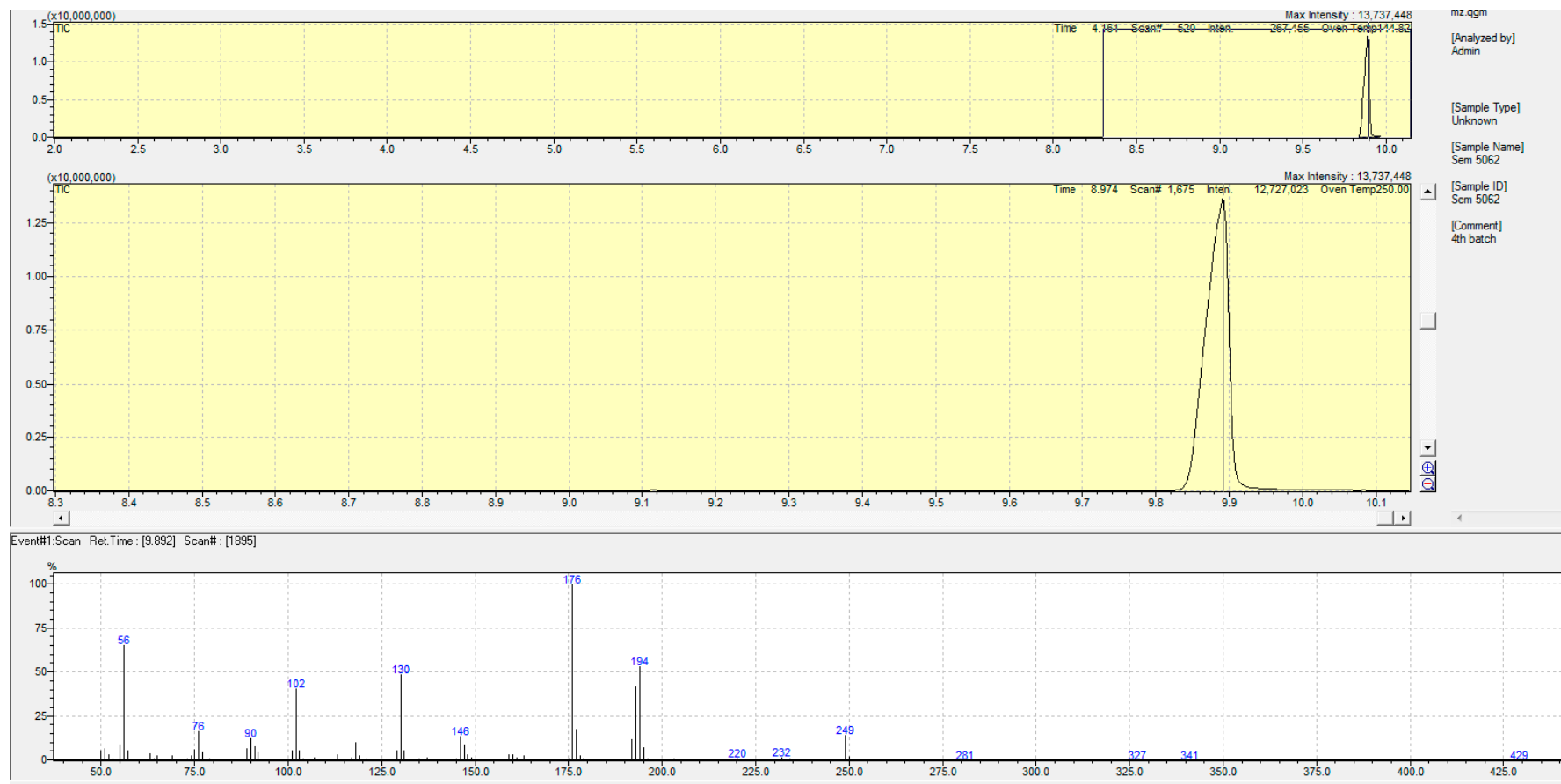


Figure S2. GC-MS data of 3-(4-nitrophenyl)acrylic acid *n*-butyl ester. $m/z = 249$.

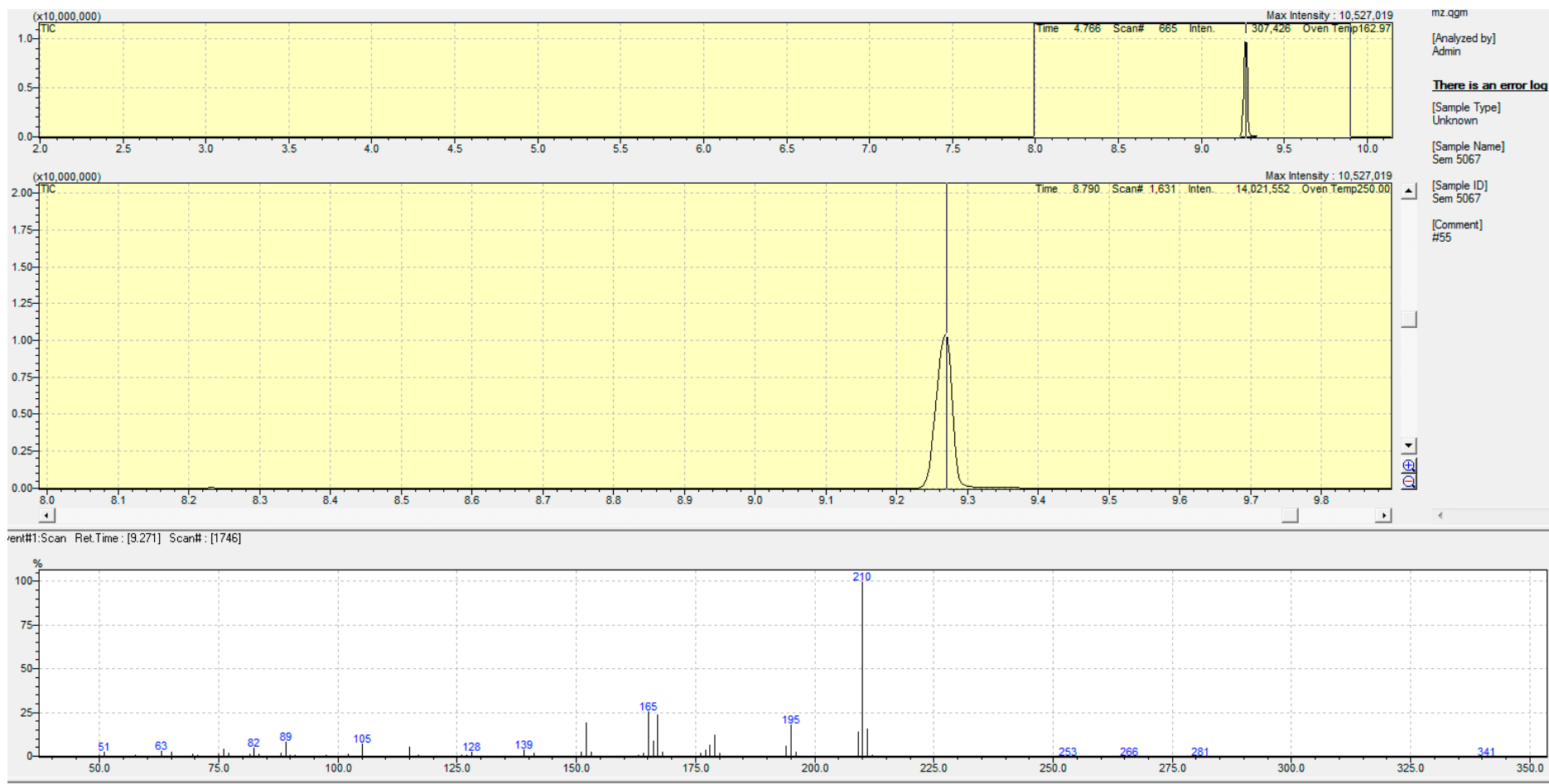


Figure S12. GC-MS data of 4-methoxystilbene. $m/z = 210$.

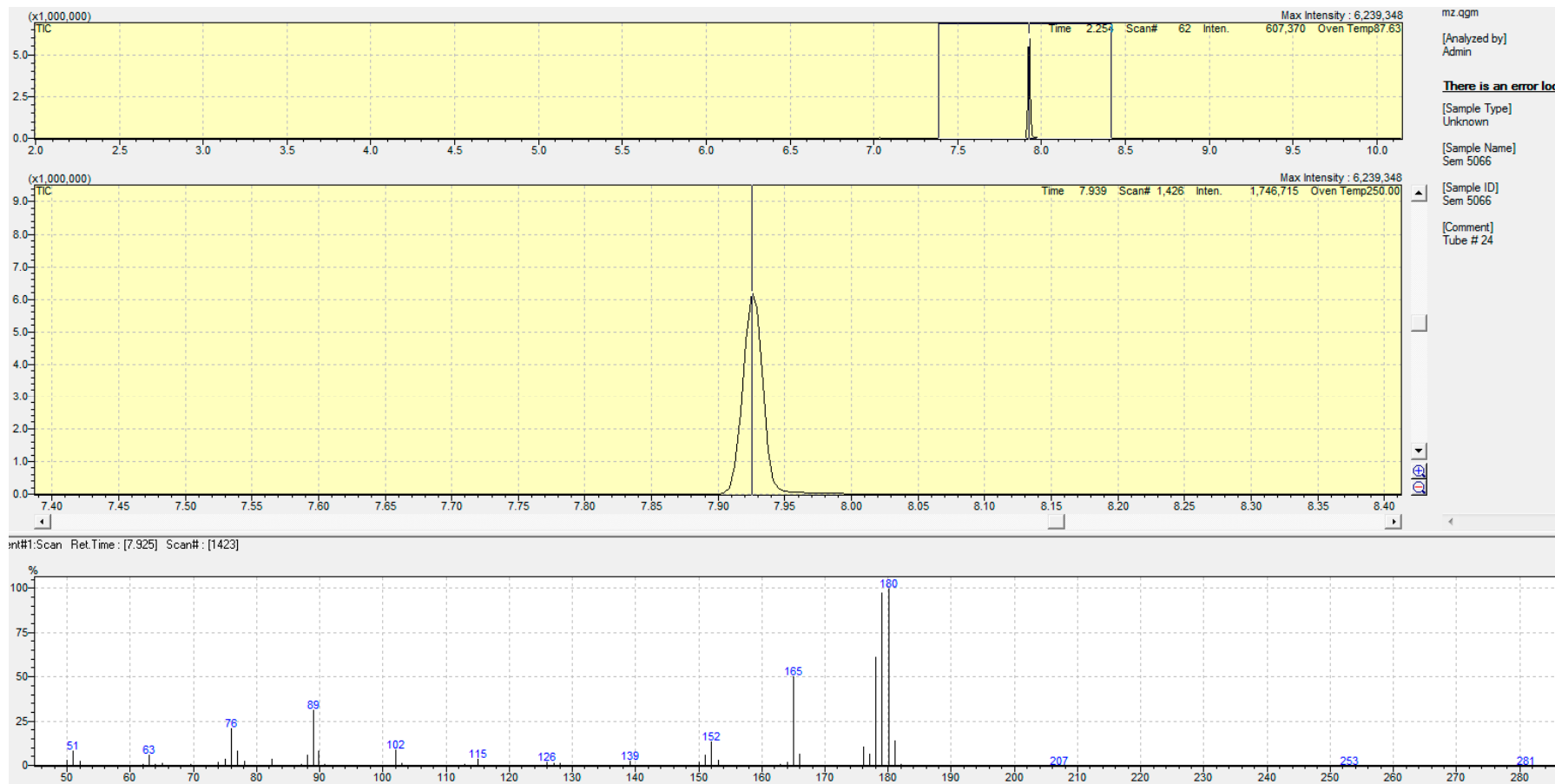


Figure S13. GC-MS data of stilbene. $m/z = 180$.

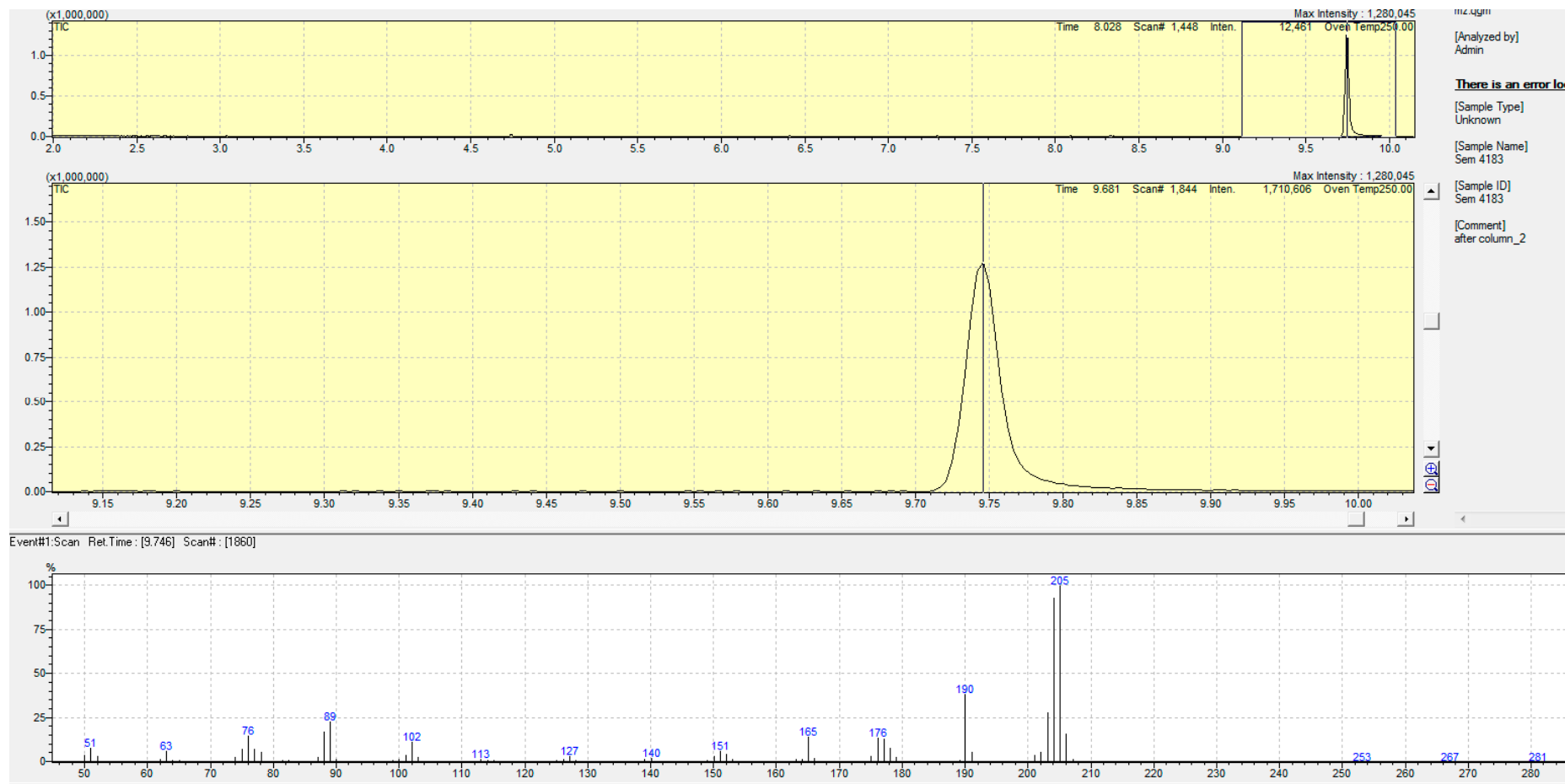


Figure S14. GC-MS data of 4-cyanostilbene. $m/z = 205$.