

Appendix K: Mass Spec Data of Reaction Mixture Components

| | PK1 | PK2 | PK3 | PK4 | PK5 | MW | Synthesis Route |
|--|-----|-----|-----|-----|-----|-----|--------------------|
| <i>e</i> -1,5-Diphenyl-2-methyl-1-pentene-4-one | 43 | 91 | 129 | 250 | 57 | 250 | P1 P3 |
| <i>z</i> -1,5-Diphenyl-2-methyl-1-pentene-4-one | 43 | 250 | 129 | 57 | 56 | 250 | P1 P3 |
| Pyrolidine | 43 | 70 | 71 | 42 | 41 | 71 | PC2 |
| <i>n</i> -Acetylamphetamine | 44 | 86 | 119 | 91 | 65 | 177 | A4 |
| Amphetamine | 44 | 91 | 43 | 42 | 65 | 135 | M5 |
| Methylenedioxyamphetamine (MDA) | 44 | 136 | 135 | 77 | 51 | 179 | MD3 |
| <i>n</i> -Methyl 1,2-(methylenedioxy)-4-(3-aminopropyl) benzene | 44 | 162 | 65 | 77 | 135 | 193 | MD5 |
| Cyclohexanone | 55 | 42 | 98 | 69 | 70 | 98 | All PC meth |
| 1,2-(Methylenedioxy)-4-(2- <i>n</i> -methylaminopropyl)-benzene | 56 | 191 | 135 | 77 | 57 | 191 | MD3 |
| Morpholine | 57 | 87 | 56 | 86 | 42 | 87 | PC3 |
| Ephedrine | 58 | 69 | 79 | 41 | 59 | 165 | M2 M3 |
| Methylenedioxymethamphetamine (MDMA) | 58 | 136 | 135 | 59 | 77 | 193 | MD3 MD5 |
| <i>n</i> -Methyl-1-[1-(hydroxy)-2-methoxy]-4-(2-aminopropyl) benzene | 58 | 51 | 77 | 137 | 94 | 195 | MD5 |
| <i>n</i> -Methyl-1-[1,2-(dimethoxy)-4-(2-aminopropyl) benzene | 58 | 152 | 51 | 151 | 59 | 209 | MD5 |
| 1-(3,4-Methylenedioxy)phenyl;-2-methoxypropane | 59 | 194 | 135 | 136 | 77 | 194 | MD5 |

| | PK1 | PK2 | PK3 | PK4 | PK5 | MW | Synthesis Route |
|---|-----|-----|-----|-----|-----|-----|------------------|
| <i>n</i> -Formylamphetamine | 72 | 44 | 118 | 91 | 65 | 163 | A1 M5 |
| <i>n,n</i> -Dimethylamphetamine | 72 | 44 | 42 | 91 | 56 | 163 | M1 M5 |
| 3,4-(Methylenedioxy)- <i>n,n</i> -dimethylamphetamine | 72 | 56 | 44 | 73 | 58 | 207 | MD3 |
| Bromobenzene | 77 | 71 | 50 | 156 | 158 | 156 | PC1A, 2A, 3A |
| Benzene | 78 | 77 | 50 | 51 | 52 | 77 | A5 |
| <i>a</i> -Methylbenzyl alcohol | 79 | 77 | 43 | 107 | 51 | 122 | |
| Piperidine | 84 | 85 | 55 | 57 | 42 | 84 | P1 |
| <i>n</i> -Formylmethamphetamine | 86 | 58 | 91 | 56 | 65 | 177 | M5 |
| 3,4-(Methylenedioxy)- <i>n,n</i> -methylethylamphetamine | 86 | 58 | 87 | 56 | 44 | 221 | MD3 |
| Phenyl-2-propanone | 91 | 134 | 92 | 43 | 65 | 134 | Numerous A and M |
| Dibenzyl ketone | 91 | 65 | 39 | 119 | 92 | 210 | Num A, M, and P |
| <i>N,n</i> -Di(<i>b</i> -phenylisopropyl)-amine | 91 | 44 | 162 | 119 | 65 | 253 | A1 M5 |
| di-(<i>b</i> -Phenylisopropyl)-methylamine | 91 | 58 | 176 | 119 | 42 | 267 | A1 M5 |
| <i>N,n</i> -Di-(<i>b</i> -phenylisopropyl)-formamide | 91 | 190 | 119 | 72 | 191 | 281 | A1 |
| <i>n</i> -(<i>b</i> -Phenylisopropyl)-benzyl methyl ketimine | 91 | 119 | 160 | 41 | 65 | 251 | A4 |
| 1-Oxy-1-phenyl-2-(<i>b</i> -phenylisopropylimino)-propane | 91 | 119 | 43 | 105 | 77 | 265 | A4 |
| 2,4-Dihydroxy-1,5-diphenyl-4-methyl-1-pentene | 91 | 159 | 131 | 65 | 115 | 268 | A4 |
| 2-Phenylmethylaziridine | 91 | 104 | 132 | 78 | 51 | 133 | A2 A3 |
| 2-Methyl-3-phenylaziridine | 91 | 132 | 42 | 105 | 92 | 133 | A2 A3 |
| Benzyl methyl ketoxime | 91 | 41 | 92 | 65 | 39 | 149 | A3 |
| Benzyl acetate | 91 | 150 | 65 | 59 | 105 | 150 | P1 |
| <i>z</i> -1,3-Diphenyl-2-methyl-1-pentene-4-one | 91 | 130 | 115 | 65 | 159 | 250 | P1 P3 |
| <i>e</i> -1,3-Diphenyl-2-methyl-1-pentene-4-one | 91 | 131 | 65 | 105 | 159 | 250 | P1 P3 |
| Isosafrole glycol | 93 | 151 | 65 | 123 | 152 | 196 | MD1 |
| Phenol | 94 | 66 | 65 | 95 | 67 | 94 | |
| Camphor | 95 | 81 | 41 | 108 | 152 | 152 | MD5 |
| 1-[1-(2-Thienyl)cyclohexyl]-piperidine | 97 | 165 | 165 | 206 | 84 | 249 | PC1B |
| 1-[1-(2-Thienyl)cyclohexyl]-morpholine | 97 | 165 | 251 | 208 | 123 | 251 | PC3B |
| 1-[3,4-(Methylenedioxy)-phenyl]-2-nitro-1-propene | 103 | 160 | 207 | 77 | 102 | 207 | MD2 |
| Phenyl nitropropene | 105 | 115 | 91 | 77 | 116 | 163 | A2 |
| 1-Phenyl-2-propanol | 105 | 106 | 77 | 79 | 91 | 136 | P6 |
| Methyl benzoate | 105 | 136 | 77 | 51 | 117 | 136 | P1 |

| | PK1 | PK2 | PK3 | PK4 | PK5 | MW | Synthesis Route |
|--|-----|-----|-----|-----|-----|-----|-----------------|
| Benzaldehyde | 106 | 105 | 77 | 51 | 63 | 106 | P1 P3 |
| 1-Morpholinocyclohexene | 108 | 81 | 167 | 109 | 152 | 167 | PC3 |
| <i>z</i> -1-Phenyl;-2-benzyl-1-propene | 115 | 208 | 91 | 193 | 134 | 208 | P1 P3 |
| 1-Phenyl-2-benzyl-2-propene | 115 | 208 | 91 | 193 | 178 | 208 | P1 P3 |
| <i>e</i> -1-Phenyl-2-benzyl-2-propene | 117 | 115 | 91 | 208 | 129 | 208 | P1 P3 |
| Dibenzyl methylamine | 120 | 91 | 42 | 77 | 102 | 211 | A1 M5 |
| 1-Cyclohexylpiperidine | 125 | 41 | 167 | | | 167 | PC1 |
| 1-Phenylcyclopentene | 129 | 44 | 43 | 128 | 115 | 129 | PC1 |
| 1-Phenylcyclohexene | 129 | 158 | 115 | 130 | 142 | 158 | PC1 |
| <i>e</i> -1,3-Diphenyl-2-methyl-2-pentene-4-one | 131 | 103 | 77 | 91 | 65 | 250 | P1 P3 |
| <i>n</i> -(<i>b</i> -Phenylisopropyl)-benzaldimine | 132 | 105 | 91 | 77 | 65 | 223 | A4 |
| 1-Phenylcyclohexanol | 133 | 105 | 176 | 55 | 120 | 176 | PC1 |
| <i>a</i> -Benzyl- <i>n</i> -methylphenethylamine | 134 | 91 | 42 | 119 | 65 | 225 | M5 |
| <i>z</i> -Phenyl-2-propanone enol acetate | 134 | 43 | 91 | 119 | 105 | 176 | P1 |
| <i>e</i> -Phenyl-2-propanone enol acetate | 134 | 91 | 43 | 119 | 105 | 176 | P1 |
| 4-Methyl-1,2-(methylenedioxy)-benzene | 135 | 136 | 77 | 79 | 51 | 136 | MD3 |
| 1,2-(Methylenedioxy)-4-propylbenzene | 135 | 77 | 164 | 51 | 79 | 164 | MD1 MD3 |
| 3,4-(Methylenedioxy)-benzyl- <i>n</i> -methylamine | 135 | 42 | 51 | 77 | 136 | 165 | MD3 |
| 3,4-(Methylenedioxy)-phenylpropanone | 135 | 77 | 51 | 43 | 178 | 178 | MD1 MD3 |
| 1-[3,4-(Methylenedioxy)]-phenyl-2-propanol | 135 | 136 | 77 | 51 | 106 | 180 | MD3 MD5 |
| 3,4-(Methylenedioxy)-benzylmethylketoxime | 135 | 178 | 176 | 77 | 136 | 283 | MD2 |
| <i>n</i> -{ <i>b</i> -[3,4-(Methylenedioxy)]-phenylmethyl}-3,4-(methylenedioxy)-benzaldimine | 135 | 178 | 176 | 77 | 136 | 283 | MD2 |
| <i>n,n</i> -di-[3,4-(Methylenedioxy)-phenylmethyl]-amine | 135 | 150 | 136 | 77 | 51 | 285 | MD2 |
| 1-[3,4(Methylenedioxy)]-4-(2-bromopropyl)-benzene | 135 | 77 | 242 | 244 | 51 | 242 | MD5 |
| 2-Thienylcyclohexene | 135 | 164 | 165 | 136 | 122 | 164 | PC1B, 2B, 3B |
| 1-Pyrrolidinocyclohexane carbonitrile | 135 | 97 | 110 | 136 | 121 | 178 | PC2 |
| 2-Methoxy-4-(2-bromopropyl)-phenol | 137 | 244 | 246 | 165 | 135 | 244 | MD5 |
| 1,2-Dimethyl-3-phenylaziridine | 146 | 105 | 42 | 132 | 91 | 147 | M2 M3 |
| Hydroxyskatole | 147 | 146 | 62 | 63 | 89 | 147 | MD2 |
| Piperonal | 149 | 150 | 121 | 63 | 65 | 150 | MD2 MD3 |
| 1-[3,4(Methylenedioxy)]-4-(3-bromopropyl)-benzene | 149 | 119 | 91 | 163 | 242 | 242 | MD5 |

| | PK1 | PK2 | PK3 | PK4 | PK5 | MW | Synthesis Route |
|--|-----|-----|-----|-----|-----|-----|-----------------|
| 1-Piperidinocyclohexyl carbonitrile (pcc) | 149 | 150 | 191 | 164 | 124 | 192 | PC1 |
| 1-Pyrrolidinocyclohexene | 150 | 151 | 122 | 136 | 95 | 151 | PC2 |
| 1-Piperidinocyclohexene | 150 | 164 | 165 | 136 | 122 | 165 | PC1 |
| 1,2-Dimethoxy-4-(2-bromopropyl)-benzene | 151 | 179 | 107 | 258 | 260 | 258 | MD5 |
| 1-Morpholinocyclohexane carbonitrile | 151 | 124 | 81 | 136 | 108 | 194 | PC3 |
| 3,4-(Methylenedioxy)-phenylmethanol | 152 | 137 | 93 | 65 | 151 | 152 | MD2 |
| 1,3-Diphenyl-2-methyl-2-pentene-4-one | 159 | 91 | 144 | 160 | 141 | 250 | P1 P3 |
| Safrole | 162 | 104 | 131 | 103 | 77 | 162 | MD1 MD3 MD5 |
| 1,2-(Dimethoxy)-4-propenylbenzene | 162 | 163 | 178 | 147 | 135 | 178 | MD3 |
| <i>n</i> -Formyl-methylenedioxyamphetamine | 162 | 135 | 72 | 44 | 77 | 207 | MD4 |
| Di-[3,4-(methylenedioxy)]-phenylpropanone | 163 | 135 | 105 | 133 | 77 | 298 | MD2 |
| <i>n</i> -{ <i>b</i> -[3,4-(Methylenedioxy)]-phenylisopropyl}-3,4-(methylenedioxy)-enzylketimine | 163 | 204 | 135 | 105 | 77 | 339 | MD2 |
| Di-[1-3,4-(methylenedioxy)-phenyl-2-propyl]-amine | 163 | 135 | 206 | 105 | 133 | 341 | MD1 |
| Di-[3,4-(methylenedioxy)-phenyl-2-propyl]-methylamine | 163 | 220 | 135 | 105 | 58 | 355 | MD1 |
| Eugenol | 164 | 77 | 55 | 103 | 149 | 164 | MD5 |
| 1,2-Dimethoxy-4-(3-bromopropyl)-benzene | 165 | 162 | 258 | 260 | 119 | 258 | MD5 |
| Diphenylmethane | 167 | 168 | 152 | 153 | 91 | 168 | P3 |
| 4-Benzylpyrimidine | 169 | 170 | 91 | 115 | 142 | 170 | |
| 4-Methyl-5-phenylpyrimide | 170 | 169 | 102 | 115 | 116 | 170 | A1 |
| <i>n</i> -{ <i>b</i> -[3,4-(Methylenedioxy)]-phenylisopropyl}-3,4-(methylenedioxy)-benzaldimine | 176 | 149 | 177 | 77 | 135 | 311 | MD2 |
| 4-Allyl-1,2-(dimethoxy)-benzene | 178 | 91 | 107 | 103 | 147 | 178 | MD5 |
| 1,2-(Dimethoxy)-4-propenylbenzene | 178 | 107 | 163 | 91 | 103 | 178 | MD5 |
| Bibenzyl | 179 | 180 | 91 | 165 | 89 | 180 | P3 |
| 1,3,5-Triphenyl-2,4,6-trimethylbenzene | 179 | 91 | 257 | 348 | 178 | 348 | P1 P3 |
| <i>Cis</i> - or <i>trans</i> -stilbene | 180 | 179 | 178 | 165 | 89 | 180 | P1 P3 |
| Trimethoxy-4-(2-bromopropyl)benzene | 181 | 209 | 288 | 290 | 148 | 277 | MD5 |
| 2-Methyl-2-phenylmethyl-5-phenyl-2,3-dihydropyrid-4-one | 186 | 91 | 158 | 143 | 187 | 277 | A1 |

| | PK1 | PK2 | PK3 | PK4 | PK5 | MW | Synthesis Route |
|---|-----|-----|-----|-----|-----|-----|-----------------|
| 1-(1-Phenylcyclohexyl)-pyrrolidine (PCPV) | 186 | 91 | 70 | 152 | 229 | 229 | PC2A |
| 1-[1-(2-Thienyl)-cyclohexyl]-pyrrolidine | 192 | 97 | 165 | 70 | 235 | 235 | PC2B |
| 1-(1-Phenylcyclohexyl)-piperidine (PCP) | 200 | 91 | 242 | 243 | 186 | 243 | PC1A |
| 1-(1-Phenylcyclohexyl)-morpholine | 202 | 91 | 245 | 244 | 117 | 245 | PC3A |
| 4-Allyl-trimethoxybenzene | 208 | 193 | 161 | 133 | 105 | 208 | MD5 |
| 1-Benzyl-3-methylnaphthalene | 232 | 217 | 108 | 215 | 202 | 232 | A1 |
| 1,3-Dimethyl-2-phenylnaphthalene | 232 | 215 | 217 | 108 | 202 | 232 | A1 |
| 4-Methyl-5-phenyl-(2-phenylmethyl)-pyridine | 258 | 259 | 243 | 244 | 260 | 259 | A1 |
| 2-Methyl-3-phenyl-6-phenylmethyl-pyridine | 258 | 259 | 180 | 244 | 260 | 259 | A1 |
| 2,4-Dimethyl-3,5-diphenylpyridine | 259 | 260 | 244 | 115 | 215 | 259 | A1 |
| 2,6-Dimethyl-3,5-diphenylpyridine | 259 | 260 | 115 | 244 | 101 | 259 | A1 |
| 2,4-Dimethyl-3-phenyl-6-phenylmethyl-pyridine | 272 | 273 | 258 | 55 | 57 | 273 | A1 |
| 2,4-Diphenyl-3,5-dimethylphenol | 274 | 259 | 101 | 165 | 152 | 274 | |

Synthesis Route Key

| | |
|-------|--|
| A1 | Amphetamine via Leuckart reaction |
| A2 | Amphetamine via benzaldehyde/nitroethane |
| A3 | Amphetamine via phenylacetone/hydroxylamine |
| A4 | Amphetamine via phenylacetone/ammonia |
| M2 M3 | Methamphetamine via ephedrine reduction |
| M5 | Methamphetamine via Leuckart reaction |
| P1 | Phenylacetone via phenylacetic acid/acetic anhydride |
| P3 | Phenylacetone via phenylacetic acid/lead acetate |
| PC1 | Piperidine/cyclohexane intermediate |
| PC1A | Phenyl addition |
| PC1B | Thionyl addition |
| PC2 | Pyrrolidine/cyclohexane intermediate |
| PC2A | Phenyl addition |
| PC2B | Thionyl addition |
| PC3 | Morpholine/cyclohexane intermediate |
| PC3A | Phenyl addition |
| PC3B | Thionyl addition |
| PK1 | Largest ion |
| PK2 | 2nd largest ion |
| PK3 | 3rd largest ion |

| | |
|-----|--------------------------------|
| PK4 | 4th largest ion |
| PK5 | 5th largest ion |
| MW | Molecular weight |
| MD2 | MDA via piperonal/nitroethane |
| MD3 | MDMA via amination of MD-P-2-P |
| MD5 | MDMA via safrole/HBr reaction |