

Compound	ESI negative spectra	EI positive spectra
DNPH	197 (4), 167 (29), 137 (100), 121 (24), 76 (27), 67 (8)	M ⁺ = 198 (75), 183 (19), 180 (19), 168 (30), 122 (53), 92 (35), 79 (100), 78 (88), 76 (66), 75 (67), 74 (28), 64 (25), 63 (45), 62 (21)
Formaldehyde-DNPH	209 (7), 181 (84), 152 (89), 122 (49), 121 (40), 120 (39), 76 (100), 67 (39)	M ⁺ = 210 (100), 180 (48), 152 (16), 122 (30), 106 (11), 92 (15), 91 (29), 90 (23), 89 (29), 80 (13), 79 (99), 78 (89), 77 (28), 76 (20), 75 (27), 74 (14), 64 (45), 63 (96), 62 (30)
Acetaldehyde-DNPH	223 (19), 193 (21), 181 (75), 164 (35), 163 (49), 152 (61), 151 (49), 122 (86), 121 (56), 120 (60), 104 (39), 76 (100), 67 (33)	M ⁺ = 224 (100), 180 (33), 152 (37), 122 (29), 104 (15), 79 (78), 78 (61), 77 (49), 63 (29)
Propionaldehyde-DNPH	237 (25), 207 (19), 181 (65), 163 (47), 152 (96), 132 (49), 122 (61), 120 (42), 104 (37), 76 (100), 72 (44), 67 (35)	M ⁺ = 238 (100), 180 (30), 152 (52), 122 (31), 92 (15), 91 (22), 90 (10), 79 (57), 78 (43), 77 (17), 76 (12), 75 (21), 64 (13), 63 (21)
Acrolein-DNPH	235 (42), 204 (19), 188 (28), 181 (51), 163 (54), 158 (86), 137 (46), 109 (40), 104 (28), 76 (65), 67 (44), 65 (100)	M ⁺ = 236 (100), 219 (13), 201 (14), 189 (48), 159 (53), 143 (24), 142 (30), 131 (15), 130 (10), 117 (22), 116 (33), 115 (23), 91 (11), 90 (16), 89 (30), 63 (30)
Butyraldehyde-DNPH	251 (24), 221 (25), 205 (14), 191 (16), 181 (39), 163 (37), 152 (100), 122 (45), 104 (31), 87 (43), 86 (29), 76 (65), 67 (25)	M ⁺ = 252 (100), 223 (6), 206 (11), 196 (13), 180 (27), 152 (60), 122 (32), 104 (12), 103 (13), 92 (15), 91 (15), 79 (43), 78 (36), 77 (23), 76 (12), 75 (21), 64 (12), 63 (20)
Isobutyraldehyde-DNPH	251 (33), 221 (12), 205 (16), 204 (16), 181 (55), 163 (61), 152 (100), 120 (45), 104 (39), 87 (82), 86 (75), 76 (100), 67 (37)	M ⁺ = 252 (100), 237 (5), 217 (13), 193 (10), 180 (34), 152 (78), 122 (52), 92 (22), 91 (20), 90 (12), 79 (58), 78 (48), 77 (31), 76 (16), 75 (38), 73 (37)
Valeraldehyde-DNPH	265 (28), 235 (18), 206 (21), 181 (28), 163 (44), 152 (100), 122 (33), 120 (35), 101 (54), 76 (56), 67 (26)	M ⁺ = 266 (70), 224 (28), 206 (100), 196 (10), 177 (9), 164 (6), 152 (20), 149 (51), 122 (31), 104 (31), 103 (37), 92 (18), 77 (32), 69 (24)

Isovaleraldehyde-DNPH	265 (35), 235 (18), 205 (21), 181 (25), 164 (33), 163 (44), 153 (46), 152 (100), 151 (39), 122 (32), 120 (23), 101 (54), 100 (35), 76 (49), 67 (26)	M^+ = 266 (100), 251 (5), 233 (8), 231 (17), 224 (25), 223 (23), 207 (18), 206 (37), 196 (35), 193 (42), 183 (28), 180 (22), 177 (23), 152 (42), 149 (29), 122 (35), 104 (27), 103 (30), 92 (20), 91 (15), 79 (31), 78 (33), 77 (42), 76 (18), 75 (27), 69 (40)
2-Oxopropanal-DNPH	432 (18), 431 (70), 251 (5), 248 (7), 182 (100), 163 (9)	433 (20), M^+ = 432 (100), 416 (11), 415 (38), 398 (3), 370 (4), 355 (4), 290 (6), 254 (12), 252 (15), 250 (69), 249 (58), 233 (15), 219 (13), 183 (77), 181 (25), 165 (11), 153 (29), 135 (11), 122 (11), 107 (12), 92 (11), 91 (23), 90 (14), 89 (12), 79 (19), 78 (20), 77 (25), 76 (15), 75 (26), 64 (17), 63 (28), 62 (15)
Benzaldehyde-DNPH	286 (12), 285 (68), 239 (12), 238 (46), 163 (47), 151 (32), 122 (30), 121 (100), 120 (88), 104 (39), 77 (28), 76 (74), 67 (23)	M^+ = 286 (100), 251 (5), 224 (5), 205 (7), 193 (11), 192 (11), 165 (22), 152 (20), 139 (12), 107 (61), 104 (20), 89 (19), 77 (44), 63 (15)
2,4-Dichlorobenzaldehyde-DNPH	357 (14), 356 (14), 355 (70), 354 (19), 353 (100), 308 (7), 306 (11), 179 (26), 163 (42), 151 (54), 145 (30), 120 (23), 104 (26), 76 (61), 67 (25)	356 (66), M^+ = 354 (100), 319 (11), 294 (6), 234 (7), 200 (19), 198 (19), 180 (18), 177 (47), 175 (82), 173 (27), 163 (26), 152 (30), 136 (19), 123 (35), 122 (16), 109 (14), 79 (45), 78 (29), 75 (20), 63 (18)
3,4-Dichlorobenzaldehyde-DNPH	357 (11), 355 (51), 353 (72), 308 (14), 306 (16), 192 (11), 191 (40), 190 (28), 189 (70), 188 (26), 179 (46), 163 (100), 152 (30), 151 (58), 147 (44), 145 (49), 134 (25), 120 (33), 105 (47), 104 (39), 76 (84), 67 (40)	356 (66), M^+ = 354 (100), 309 (3), 307 (3), 294 (11), 292 (9), 235 (5), 234 (6), 233 (5), 226 (8), 200 (15), 198 (16), 180 (16), 177 (22), 175 (44), 174 (18), 173(27), 172 (17), 163 (22), 152 (22), 147 (19), 145 (23), 123 (27), 122 (13), 109 (14), 79 (37), 78 (26), 75 (19), 63 (14)
5-Methyl-2-furfural-DNPH	290 (16), 289 (96), 242 (60), 182 (32), 181 (41), 163 (63), 125 (47), 120 (40), 104 (33), 76 (100), 67 (37), 60 (32)	291 (15), M^+ = 290 (100), 200 (5), 169 (6), 154 (4), 136 (5), 115 (12), 111 (31), 109 (15), 79 (17), 75 (5), 63 (5)
5-Bromosalicylaldehyde-DNPH	381 (33), 379 (32), 217 (12), 216 (11), 215 (12), 182 (100), 163 (30), 151 (23),	383 (16), 382 (99), 381 (17), M^+ = 380 (100), 365 (5), 363 (5), 322 (8), 320

	120 (7), 104 (9), 76 (19), 67 (11)	(15), 318 (8), 203 (45), 202 (24), 201 (63), 200 (33), 199 (57), 198 (13), 197 (39), 185 (14), 183 (34), 181 (15), 180 (22), 173 (11), 171 (35), 169 (27), 167 (10), 154 (9), 153 (30), 152 (39), 151 (11), 145 (10), 143 (11), 122 (9), 92 (12), 91 (20), 90 (18), 79 (21), 78 (18), 77 (18), 76 (17), 75 (20), 65 (10), 64 (20), 63 (41), 62 (13)
Glyoxal-diDNPH	417 (31), 234 (10), 182 (100)	419 (19), M ⁺ = 418 (100), 401 (19), 384 (5), 356 (6), 341 (3), 238 (15), 236 (65), 235 (55), 219 (17), 205 (18), 183 (63), 181 (15), 165 (14), 164 (12), 153 (28), 91 (21), 90 (18), 89 (14), 79 (21), 78 (20), 77 (25), 76 (19), 75 (33), 64 (19), 63 (35), 62 (19)
Glutaraldehyde-diDNPH	460 (9), 459 (30), 279 (9), 263 (18), 235 (25), 223 (30), 197 (49), 182 (100), 179 (98), 163 (53), 153 (35), 152 (39), 151 (33), 137 (28), 120 (21), 112 (16), 76 (25), 67 (11)	M ⁺ = 460 (7), 280 (7), 264 (34), 263 (100), 262 (12), 231 (12), 217 (18), 203 (14), 189 (11), 183 (27), 168 (11), 167 (11), 164 (23), 153 (16), 152 (15), 122 (17), 104 (10), 103 (13), 95 (10), 92 (15), 91 (17), 90 (14), 80 (18), 79 (26), 78 (21), 77 (23), 76 (16), 75 (23), 68 (11), 67 (26), 65 (13), 64 (15), 63 (31), 62 (12)
Acetone-DNPH	237 (72), 207 (72), 181 (46), 178 (67), 164 (56), 151 (44), 132 (100), 121 (35), 104 (26), 76 (53)	M ⁺ = 238 (100), 222 (4), 196 (5), 181 (38), 180 (23), 152 (56), 135 (13), 122 (32), 115 (28), 91 (24), 79 (64), 78 (55), 77 (25), 76 (15), 75 (23)
2-Pentanone-DNPH	265 (44), 235 (28), 219 (11), 206 (12), 178 (32), 152 (100), 122 (23), 76 (18)	267 (40), M ⁺ = 266 (100), 231 (23), 219 (23), 196 (20), 191 (20), 183 (20), 181 (47), 180 (28), 178 (27), 165 (24), 152 (51), 149 (20), 122 (27), 104 (20), 87 (61), 79 (28), 78 (30), 77 (24), 69 (23), 63 (20)

3-Pentanone-DNPH	265 (33), 235 (19), 219 (11), 206 (12), 192 (19), 178 (33), 168 (12), 153 (25), 152 (100), 151 (14), 138 (11), 122 (26), 76 (14), 67 (5)	267 (31), M ⁺ = 266 (100), 231 (19), 205 (23), 181 (68), 180 (20), 165 (20), 152 (51), 122 (22), 87 (90), 79 (31), 78 (32), 69 (34), 63 (25)
3-Methyl-2-butanone-DNPH	265 (40), 235 (21), 192 (9), 181 (12), 164 (21), 152 (100), 122 (23), 104 (5), 76 (14), 67 (5)	M ⁺ = 266 (100), 233 (13), 231 (12), 185 (11), 181 (16), 165 (13), 152 (19), 122 (14), 87 (35), 79 (13), 78 (14), 77 (12), 75 (13), 69 (19)
3-Hexanone-DNPH	279 (30), 249 (18), 233 (5), 220 (9), 206 (11), 192 (23), 178 (14), 168 (12), 153 (26), 152 (100), 122 (23), 76 (7), 67 (4)	281 (32), M ⁺ = 280 (100), 245 (29), 219 (12), 217 (10), 205 (25), 199 (13), 183 (18), 181 (47), 180 (16), 165 (29), 152 (28), 122 (14), 101 (39), 79 (14), 78 (16), 77 (12), 75 (12), 71 (14), 70 (22), 63 (14)
3-Methyl-2-hepten-6-one-DNPH	305 (23), 236 (7), 219 (4), 206 (4), 178 (9), 153 (16), 152 (100), 151 (11), 138 (5), 122 (19), 104 (4), 76 (9)	M ⁺ = 306 (8), 289 (33), 260 (13), 248 (22), 233 (12), 231 (40), 207 (12), 205 (22), 196 (46), 191 (58), 190 (12), 177 (13), 152 (11), 150 (9), 109 (23), 83 (16), 82 (100), 81 (16), 69 (96), 67 (34)
Cyclopentanone-DNPH	263 (40), 234 (18), 233 (100), 218 (14), 217 (74), 204 (14), 203 (28), 181 (19), 153 (18), 152 (54), 151 (26), 138 (16), 122 (16), 121 (18), 120 (21), 104 (14), 76 (33), 67 (16)	265 (27), M ⁺ = 264 (83), 248 (4), 230 (9), 229 (5), 180 (22), 173 (11), 152 (65), 131 (13), 128 (13), 122 (28), 85 (100), 79 (43), 78 (37), 67 (57)
2-Cyclohexen-1-one-DNPH	276 (16), 275 (100), 245 (25), 229 (28), 181 (12), 170 (23), 168 (19), 152 (19), 138 (14), 122 (11), 95 (7), 76 (14), 62 (9)	277 (26), M ⁺ = 276 (100), 241 (15), 230 (6), 195 (7), 185 (7), 184 (7), 183 (9), 168 (9), 167 (10), 157 (8), 156 (8), 155 (8), 154 (10), 153 (10), 152 (11), 128 (9), 115 (7), 97 (92), 79 (30), 78 (16), 77 (33), 67 (30)
2-Hydroxy-3-methyl-2-cyclopentenone-DNPH	291 (46), 244 (7), 183 (14), 182 (100), 181 (16), 153 (18), 152 (56), 122 (18), 108 (9), 76 (9) 374 (28), 373 (100), 343 (4), 168 (16), 153 (32), 152 (68)	293 (15), M ⁺ = 292 (100), 183 (15), 153 (11), 109(16), 82 (22), 69 (88), 63 (10)

Dicyclohexylketone-DNPH	374 (28), 373 (100), 343 (4), 168 (16), 153 (32), 152 (68)	375 (23), M ⁺ = 374 (100), 357 (6), 340 (16), 339 (64), 319 (32), 291 (12), 273 (10), 271 (11), 259 (15), 257 (23), 231 (11), 230 (27), 229 (11), 208 (12), 184 (12), 177 (13), 136 (12), 110 (21), 109 (25), 108 (18), 95 (36), 83 (76), 81 (47), 79 (20), 67 (31)
L-Carvone-DNPH	330 (21), 329 (100), 270 (9)	M ⁺ = 330 (56), 290 (24), 289 (100), 253 (6), 249 (5), 207 (6), 133 (8), 132 (8), 131 (9), 107 (17), 106 (12), 105 (14), 93 (11), 91 (25), 79 (18), 77 (15)
D-Camphor-DNPH	332 (25), 331 (100), 181 (7), 152 (14), 135 (7), 76 (7)	333 (35), M ⁺ = 332 (100), 315 (8), 297 (22), 289 (41), 271 (21), 255 (10), 243 (8), 209 (6), 197 (4), 196 (6), 195 (4), 169 (3), 168 (5), 167 (6), 153 (20), 134 (14), 133 (12), 109 (20), 108 (15), 107 (39), 106 (28), 105 (11), 95 (13), 94 (12), 93 (26), 91 (23), 81 (20), 79 (32), 77 (20), 69 (22), 67 (22)
a-Ionone-DNPH	372 (25), 371 (100), 218 (19), 152 (11), 76 (4)	373 (20), M ⁺ = 372 (90), 357 (18), 337 (10), 317 (18), 316 (100), 302 (10), 301 (58), 289 (19), 282 (17), 281 (47), 255 (13), 254 (19), 253 (14), 249 (12), 242 (12), 235 (19), 229 (22), 216 (16), 208 (21), 135 (18), 134 (64), 122 (34), 119 (41), 107 (55), 105 (24), 93 (78), 91 (64), 79 (28), 77 (40)
Acetovanillon- DNPH	346 (21), 345 (100), 315 (7), 300 (9), 183 (16), 182 (91), 168 (19), 152 (28), 151 (30), 137 (21), 120 (11), 109 (23), 76 (25), 67 (11)	347 (21), M ⁺ = 346 (100), 331 (10), 312 (15), 299 (8), 285 (24), 284 (38), 283 (21), 268 (34), 238 (10), 210 (7), 194 (15), 166 (15), 165 (21), 164 (25), 151 (18), 149 (39), 135 (10), 123 (14), 77 (11)
4-Acetylbenzoic acid-DNPH	344 (21), 343 (100), 299 (5), 282 (11), 269 (19), 254 (7), 223 (9), 182 (77), 163 (18), 152 (32), 151 (23), 136 (23), 119 (12), 76 (26), 69 (11), 67 (7)	345 (28), M ⁺ = 344 (100), 327 (12), 297 (13), 281 (13), 265 (35), 250 (11), 236 (6), 207 (6), 206 (7), 205 (6), 178 (19), 165 (34), 162 (24), 152 (13), 148 (11), 147 (34), 131 (10), 121 (14), 103 (16), 77 (14), 65 (18)

2-Acetylfuran- DNPH	290 (18), 289 (100), 259 (25), 184 (39), 168 (21), 151 (28), 138 (21), 120 (14), 104 (7), 76 (25), 69 (14), 67 (7)	M^+ = 290 (100), 260 (2), 199 (2), 198 (2), 197 (2), 181 (2), 171 (2), 170 (3), 169 (5), 168 (6), 149 (9), 141 (2), 140 (3), 139 (4), 136 (4), 115 (13), 111 (26), 108 (10), 94 (11), 93 (34), 66 (10), 65 (13)
Acetophenone- DNPH	300 (20), 299 (100), 254 (46), 151 (36), 76 (41)	M^+ = 300 (100), 265 (28), 253 (9), 219 (12), 207 (10), 192 (8), 178 (19), 166 (11), 152 (10), 121 (26), 118 (18), 103 (45), 77 (56)
3-Aminoaceto-phenone- DNPH	315 (19), 314 (100), 269 (53), 251 (12), 181 (14), 179 (12), 168 (19), 151 (40), 138 (11), 134 (23), 120 (14), 104 (9), 76 (28), 67 (11)	316 (16), M^+ = 315 (100), 298 (7), 281 (40), 280 (57), 268 (16), 267 (10), 226 (21), 222 (25), 221 (27), 220 (11), 207 (10), 206 (7), 181 (14), 180 (17), 118 (24), 92 (30), 91 (14), 65 (21)
4-Methoxyaceto- phenone-DNPH	330 (23), 329 (100), 314 (5), 284 (40), 256 (11), 205 (12), 179 (14), 168 (19), 151 (44), 76 (39), 67 (12)	331 (17), M^+ = 330 (100), 281 (22), 268 (7), 222 (6), 194 (7), 165 (10), 151 (15), 148 (17), 135 (20), 134 (12), 133 (36), 107 (7), 92 (8), 91 (8), 77 (14)
2',4'-Dihydroxy- acetophenone- DNPH	332 (14), 331 (74), 284 (7), 256 (7), 182 (100), 179 (21), 151 (21), 148 (16), 134 (16), 109 (7), 76 (12), 67 (5)	333 (17), M^+ = 332 (100), 315 (14), 285 (4), 210 (5), 196 (5), 183 (5), 153 (13), 150 (18), 137 (10), 136 (12), 135 (67), 107 (25), 81 (11), 77 (11)
Benzophenone-DNPH	362 (26), 361 (100), 255 (16), 126 (25), 101 (28), 89 (33), 76 (26)	M^+ = 362 (100), 327 (42), 315 (11), 281 (10), 268 (18), 239 (15), 180 (32), 165 (27), 139 (4), 105 (11), 77 (26)