

Supporting Tables and Figures for article

HPLC–HR-ESI–MS/MS identification of fluorescent dyes and optical brighteners and their degradation products in daylight fluorescent paints

Lukas Reiß^{1,2} – ORCID: 0000-0003-3930-7387

Susanne Machill¹ – ORCID: 0000-0003-0255-0391

Tilo Lübken³ – ORCID: 0000-0003-3383-9518

Christoph Herm² – ORCID: 0000-0001-9579-535X

Correspondence: Lukas Reiß – lukas.reiss@tu-dresden.de

1 – Chair of Bioanalytical Chemistry, Technische Universität Dresden, Bergstraße 66, 01069 Dresden, Germany

2 – Laboratory of Archaeometry, Dresden University of Fine Arts, Güntzstraße 34, 01307 Dresden, Germany

3 – Chair of Organic Chemistry I, Technische Universität Dresden, Bergstraße 66, 01069 Dresden, Germany

Table S1: Synonyms and Identifiers of the dyes and optical brighteners used in the study; retention times and fragmentation patterns of the dyes and optical brighteners determined by HPLC–HR-MS/MS

Abbreviation	Synonyms and Identifiers	RT / min	Exact Mass (Formula)	Fragments (Loss)*	Intensity ratio
BV11	Basic Violet 11 Rhodamine 3B C.I. 45175 CAS 2390-63-8	24.1	471.2642 (C ₃₀ H ₃₅ N ₂ O ₃ ⁺)	471.2647 443.2340 (C ₂ H ₄) 427.2020 (C ₃ H ₈) 413.1875 (C ₄ H ₁₀) 399.1713 (C ₅ H ₁₂) 385.1673 (C ₅ H ₁₂ N) 383.1382 (C ₆ H ₁₆) 371.1465 (C ₆ H ₁₄ N/C ₇ H ₁₆)** 369.1952 (C ₅ H ₁₀ O ₂) 369.1245 (C ₇ H ₁₈) 355.1796 (C ₆ H ₁₂ O ₂) 355.1080 (C ₈ H ₂₀)	1.2 37.9 7.7 7.8 100 4.3 0.7 2.7 0.1 1.3 0.4 10.8
BV11:1	Basic Violet 11:1 Rhodamine 3B-SPL C.I. 45174 CAS 73398-89-7	23.3	457.2486 (C ₂₉ H ₃₃ N ₂ O ₃ ⁺)	457.2495 441.2174 (CH ₄) 427.2022 (C ₂ H ₆) 413.1868 (C ₃ H ₈) 399.1833 (C ₃ H ₈ N) 397.1547 (C ₄ H ₁₂) 385.1604 (C ₄ H ₁₀ N/C ₅ H ₁₂)** 383.1393 (C ₅ H ₁₄) 369.1243 (C ₆ H ₁₆) 355.1205 (C ₆ H ₁₆ N) 341.1047 (C ₇ H ₁₈ N)	9.1 0.9 6.2 100 6.1 0.7 3.4 3.1 22.7 2.1 0.7
RhB	Rhodamine B C.I. 45170 CAS 81-88-9	21.2	443.2329 (C ₂₈ H ₃₁ N ₂ O ₃ ⁺)	443.2334 427.2020 (CH ₄) 413.1864 (C ₂ H ₆) 399.1711 (C ₃ H ₈) 385.1674 (C ₃ H ₈ N)	8.3 0.9 6.6 100 6.2

				383.1388 (C ₄ H ₁₂) 371.1453 (C ₄ H ₁₀ N/C ₅ H ₁₂)** 369.1960 (C ₃ H ₆ O ₂) 369.1238 (C ₅ H ₁₄) 355.1806 (C ₄ H ₈ O ₂) 355.1084 (C ₆ H ₁₆) 341.1047 (C ₆ H ₁₆ N) 327.1520 (C ₆ H ₁₂ O ₂) 327.0893 (C ₇ H ₁₈ N)	0.8 3.8 0.1 3.2 1.0 24.2 2.0 0.1 1.0
SRB	Sulforhodamine B Acid Red 52 C.I. 45100 CAS 3520-42-1	16.3	559.1567 (C ₂₇ H ₃₀ N ₂ O ₇ S ₂ +H ⁺)	559.1568 543.1234 (CH ₄) 531.1232 (C ₂ H ₄) 529.1086 (C ₂ H ₆) 515.0944 (C ₃ H ₈) 501.0892 (C ₃ H ₈ N) 487.0680 (C ₄ H ₁₀ N/C ₅ H ₁₂)** 479.1983 (O ₃ S) 477.1857 (H ₂ O ₃ S) 471.0313 (C ₆ H ₁₆)	59.9 1.9 4.8 8.1 100 5.3 4.0 4.1 3.2 9.4
Rh6G	Rhodamine 6G C.I. 45160 CAS 989-38-8	21.7	443.2329 (C ₂₈ H ₃₁ N ₂ O ₃ ⁺)	443.2335 415.2019 (C ₂ H ₄) 399.1697 (C ₃ H ₈) 386.1626 (C ₄ H ₉) 371.2126 (C ₃ H ₄ O ₂) 371.1481 (C ₄ H ₁₀ N/C ₅ H ₁₂)** 357.1229 (C ₆ H ₁₄) 341.1649 (C ₅ H ₁₀ O ₂) 327.1504 (C ₆ H ₁₂ O ₂) 313.1330 (C ₇ H ₁₄ O ₂)	7.6 100 2.5 20.0 0.7 2.7 4.0 12.0 3.0 2.2
BR1:1	Basic Red 1:1 Rhodamine 6GD C.I. 45161 CAS 3068-39-1	20.6	429.2173 (C ₂₇ H ₂₉ N ₂ O ₃ ⁺)	429.2175 413.1860 (CH ₄) 400.1771 (C ₂ H ₅) 386.1732 (C ₂ H ₅ N) 385.1592 (C ₂ H ₆ N/C ₃ H ₈)** 371.1393 (C ₄ H ₁₀) 355.1788 (C ₃ H ₆ O ₂) 355.1443 (C ₄ H ₁₀ O) 341.1648 (C ₄ H ₈ O ₂) 327.1493 (C ₅ H ₁₀ O ₂) 312.1305 (C ₆ H ₁₃ O ₂) 298.1162 (C ₇ H ₁₅ O ₂ /C ₆ H ₁₃ NO ₂) 284.1070 (C ₇ H ₁₅ NO ₂)	25.8 9.0 8.3 6.4 5.8 9.7 3.6 5.4 68.3 100 18.5 10.4 4.0
Rh575	Rhodamine 575 CAS 25152-49-2	19.0	415.2016 (C ₂₆ H ₂₆ N ₂ O ₃ +H ⁺)	415.2021 399.1709 (CH ₄) 386.1630 (C ₂ H ₅) 371.2115 (CO ₂) 371.1456 (C ₂ H ₆ N/C ₃ H ₈)** 357.1246 (C ₄ H ₁₀)	21.5 12.7 35.9 1.0 11.7 42.1

				341.1658 (C ₃ H ₆ O ₂) 326.1514 (C ₃ H ₇ NO ₂) 313.1337 (C ₅ H ₁₀ O ₂) 297.1141 (C ₅ H ₁₂ NO ₂) 285.1146 (C ₆ H ₁₂ NO ₂)	100 14.2 52.7 12.4 8.1
SY172	Solvent Yellow 172 CAS 68427-35-0	20.7	414.1118 (C ₂₀ H ₁₉ N ₃ O ₅ S+H ⁺)	414.1114 398.0802 (CH ₄) 386.0813 (C ₂ H ₄) 384.0606 (C ₂ H ₆) 370.0483 (C ₃ H ₈) 356.0474 (C ₃ H ₈ N) 334.1313 (H ₂ NO ₂ S) 319.1087 (CH ₅ NO ₂ S) 306.0979 (C ₂ H ₆ NO ₂ S) 290.0699 (C ₃ H ₁₀ NO ₂ S)	63.1 3.5 2.2 5.7 100 6.5 52.2 7.0 5.5 15.3
SY44	Solvent Yellow 44 Disperse Yellow 11 Solvent Yellow 135? [8]*** C.I. 56200 CAS 2478-20-8 CAS 144246-02-6	20.1	317.1285 (C ₂₀ H ₁₆ N ₂ O ₂ +H ⁺)	317.1289 274.1213 (CHNO) 225.0656 (C ₇ H ₈) 213.0650 (C ₈ H ₈) 195.0552 (C ₈ H ₁₀ O) 170.0600 (C ₉ H ₉ NO) 167.0598 (C ₉ H ₁₀ O ₂) 142.0645 (C ₁₀ H ₉ NO ₂) 140.0478 (C ₁₀ H ₁₁ NO ₂) 115.0542 (C ₁₁ H ₁₀ N ₂ O ₂) 105.0697 (C ₁₂ H ₈ N ₂ O ₂) 103.0544 (C ₁₂ H ₁₀ N ₂ O ₂) 79.0541 (C ₁₄ H ₁₀ N ₂ O ₂) 77.0384 (C ₁₂ H ₁₂ N ₂ O ₂)	38.3 3.0 8.4 5.5 58.7 23.1 10.9 11.3 4.2 5.6 100 8.1 18.7 9.0
BY40	Basic Yellow 40 CAS 29556-33-0	15.4	362.1863 (C ₂₂ H ₂₄ N ₃ O ₂ ⁺)	362.1863 346.1551 (CH ₄) 332.1392 (C ₂ H ₆) 318.1242 (C ₃ H ₈) 304.1209 (C ₃ H ₈ N) 302.0926 (C ₄ H ₁₂) 290.1279 (C ₄ H ₈ O) 290.1046 (C ₄ H ₁₀ N) 275.1056 (C ₅ H ₁₁ O) 275.0786 (C ₅ H ₁₃ N)	1.3 1.0 7.9 100 8.8 4.6 6.7 4.4 3.3 0.2
FB184	Fluorescent Brightener 184 C.I. 515245 CAS 12224-40-7	49.0	431.1788 (C ₂₆ H ₂₆ N ₂ O ₂ S+H ⁺)	431.1783 415.1477 (CH ₄) 401.1306 (C ₂ H ₆) 399.1162 (C ₂ H ₈) 385.1001 (C ₃ H ₁₀) 374.1080 (C ₄ H ₉)	8.8 100 15.9 18.6 5.4 4.9
FB61	Fluorescent Brightener 61 Coumarin 1 C.I. 551100 CAS 91-44-1	22.5	232.1332 (C ₁₄ H ₁₇ NO ₂ +H ⁺)	232.1336 203.0945 (C ₂ H ₅) 188.0708 (C ₃ H ₈) 175.0993 (C ₃ H ₅ O) 175.0628 (C ₄ H ₉) 160.1108 (C ₃ H ₄ O ₂) 160.0758 (C ₄ H ₈ O)	20.5 100 86.5 16.4 2.0 0.9 10.8

				160.0502 (C ₄ H ₁₀ N)	0.2
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*Fragmentation Energy: 50 eV for BV11, BV11:1, RhB, SRB, Rh6G (peak at 21.2 min), BR1:1, Rh575, BY40, FB184, 40 eV for Rh6G, SY172, 30 eV for SY44, 20 eV for FB61; **The peaks could not be resolved, but were clarified in [28]; ***There is contradictory information regarding Solvent Yellow 135. Fremout and Saverwyns refer to the product name “Alberta Yellow” used by DayGlo Color Corp. as the coumarin dye Solvent Yellow 135 [5], which is also stated in US Patent 6211941 (Erland J, inventor. Matte process for composite photography. USA patent 6221941. 1997 April 3). This information was relied upon by Schmidtke Sobeck et al. [8], who assumed that it could not be distinguished from SY172 by Raman spectroscopy because coumarin dyes have similar Raman spectra. However, Schmidtke Sobeck et al. [8] state for Solvent Yellow 135 CAS 144246-02-6 as well as a neutral mass of 316 g/mol neither of which leads to a coumarin dye, but to an aminonaphthalimide dye that has the same structure as the SY44 used in the present study. Accordingly, it can also be distinguished from SY172 by Raman spectroscopy. It seems that there are two CAS numbers for this aminonaphthalimide and that the term Solvent Yellow 135 was given to two different dyes, once to the aminonaphthalimide and once as a synonym for SY172.

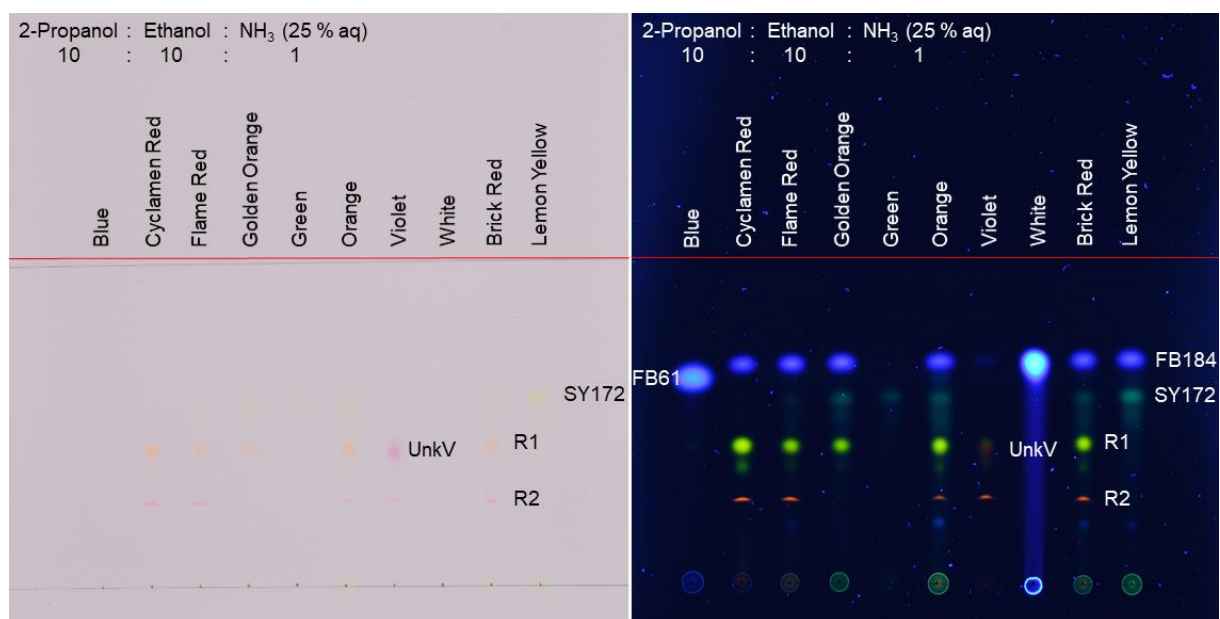


Figure S1: TLC separation of the DFPs from Kremer Pigmente

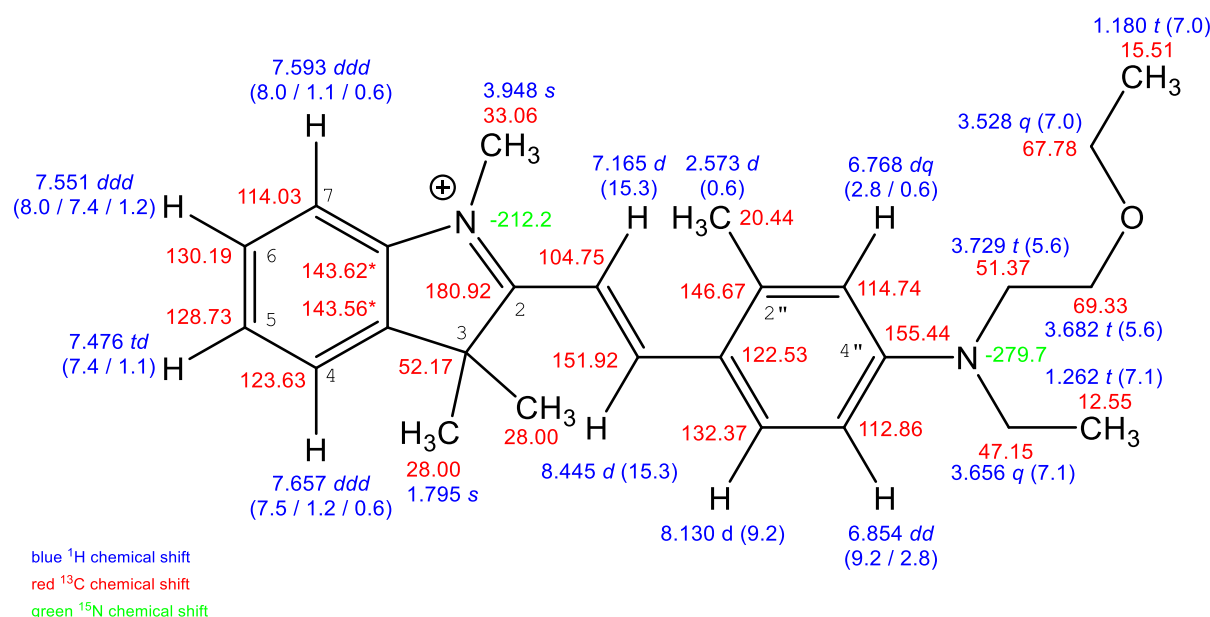


Figure S2: Chemical structure of UnkV with ^1H , ^{13}C and ^{15}N signal assignment

Characterization: 2-(2-{4-[(2-Ethoxy-ethyl)-ethyl-amino]-2-methyl-phenyl}-vinyl)-1,3,3-trimethyl-3H-indolium

The ^1H NMR spectrum (Figure S3) consists of 9 well resolved signals in the aromatic region, each integrating for one proton. The $^{13}\text{C}\{^1\text{H}\}$ and DEPT135 spectra are shown in Figure S4. A *trans*-configured double bond, an *ortho*-substituted aromatic ring and an 1,2,4-trisubstituted aromatic ring were identified by analyzing the coupling pattern and interpreting the COSY spectrum (Figure S5). In addition, the ^1H spectrum shows four methyl groups, two ethyl groups and one ethylene group. HMBC correlations revealed that the *ortho*-substituted aromatic ring is part of an indole system with two methyl groups in 3-position and an additional N-methylation (Figure S6). The *trans*-configured double bond links the indole system to the trisubstituted aromatic ring, which carries a methyl group in the 2''-position. There is an amino group at 4''-position of this aromatic ring, which is further N-ethylated and N-ethoxyethylated. $^1\text{H}/^{15}\text{N}$ -HMBC and HSQC experiments support this structural proposal (Figures S7 and S8).

NMR signals: ^1H NMR (600.2 MHz, CH_3OD): δ_{H} = 8.445 (*d*, J = 15.3 Hz, 1 H), 8.130 (*d*, J = 9.2 Hz, 1 H), 7.657 (*ddd*, J = 7.5, 1.2, 0.6 Hz, 1 H), 7.593 (*ddd*, J = 8.0, 1.1, 0.6 Hz, 1 H), 7.551 (*ddd*, J = 8.0, 7.4, 1.2 Hz, 1 H), 7.476 (*td*, J = 7.4, 1.1 Hz, 1 H), 7.165 (*d*, J = 15.3 Hz, 1 H), 6.854 (*dd*, J = 9.2, 2.8 Hz, 1 H), 6.768 (*dq*, J = 2.8, 0.6 Hz, 1 H), 3.948 (*s*, 3 H), 3.729 (*t*, J = 5.6 Hz, 2 H), 3.682 (*t*, J = 5.6 Hz, 2 H), 3.656 (*q*, J = 7.1, 2 H), 3.525 (*q*, J = 7.0 Hz, 2 H), 2.573 (*d*, J = 0.6 Hz, 3 H), 1.795 (*s*, 6 H), 1.262 (*t*, J = 7.1 Hz, 3 H), 1.180 (*t*, J = 7.0 Hz, 3 H) ppm; ^{13}C NMR (150.9 MHz, CH_3OD): δ_{C} = 180.92, 155.44, 151.92, 146.67, 143.62, 143.56, 132.37, 130.19, 128.73, 123.63, 122.53, 114.74, 114.03, 112.86, 104.75, 69.33, 67.78, 52.17, 51.37, 47.15, 33.06, 28.00, 20.44, 15.51, 12.55 ppm; ^{15}N NMR (60.8 MHz, CH_3OD): $\delta(^{15}\text{N})$ = -212.2, -279.7 ppm.

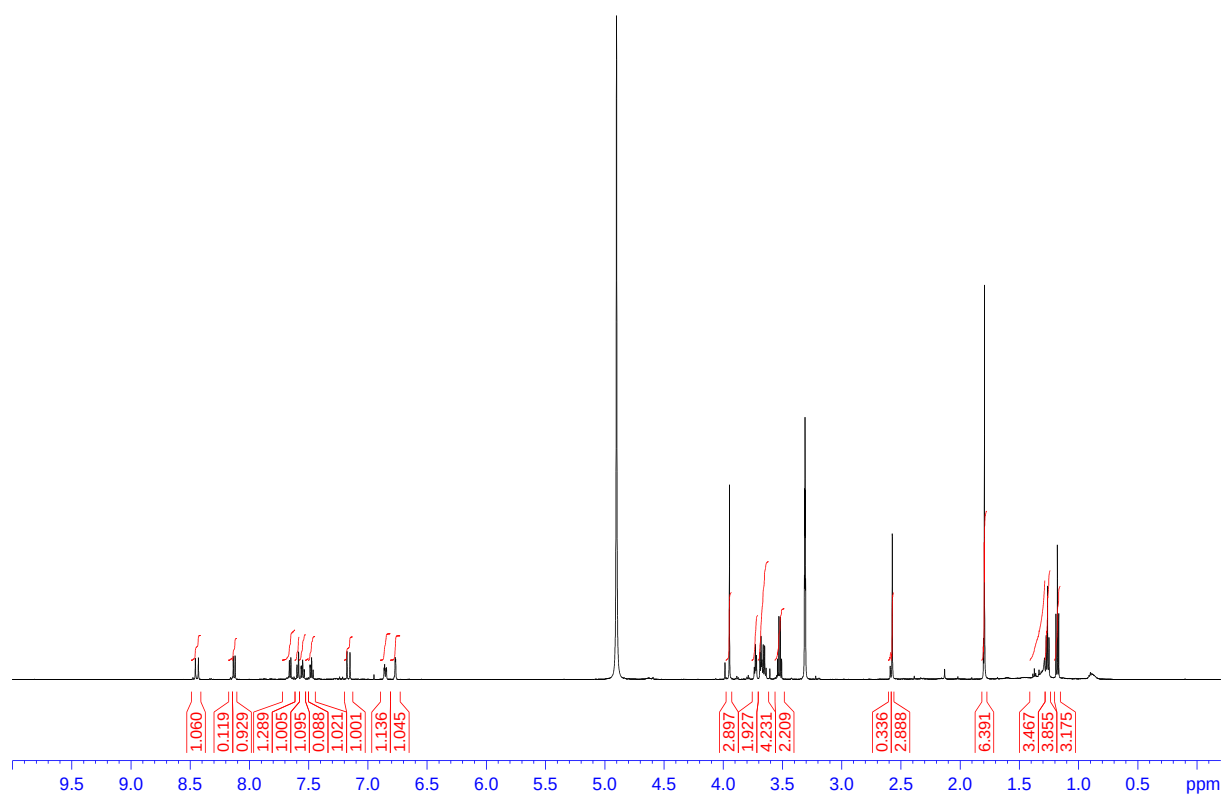


Figure S3: ^1H NMR spectrum (600 MHz, CD_3OD) of UnkV

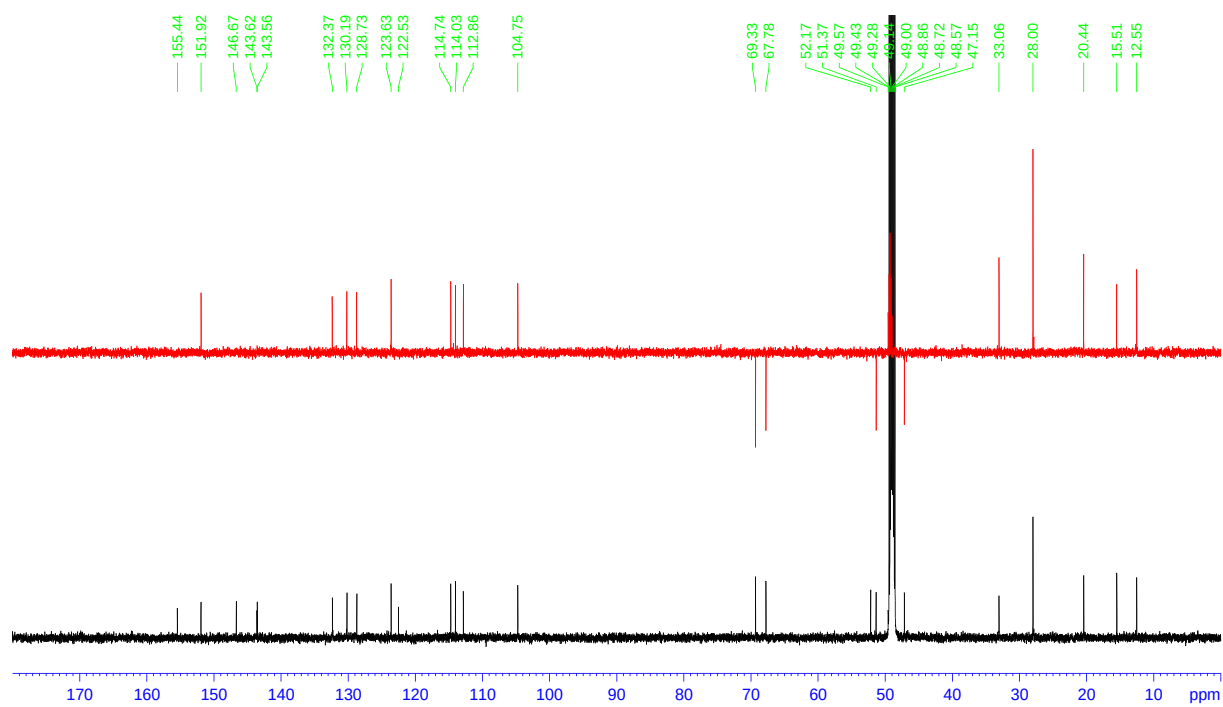


Figure S4: $^{13}\text{C}\{^1\text{H}\}$ (bottom) and DEPT135 (top) NMR spectra (150 MHz, CD_3OD) of UnkV

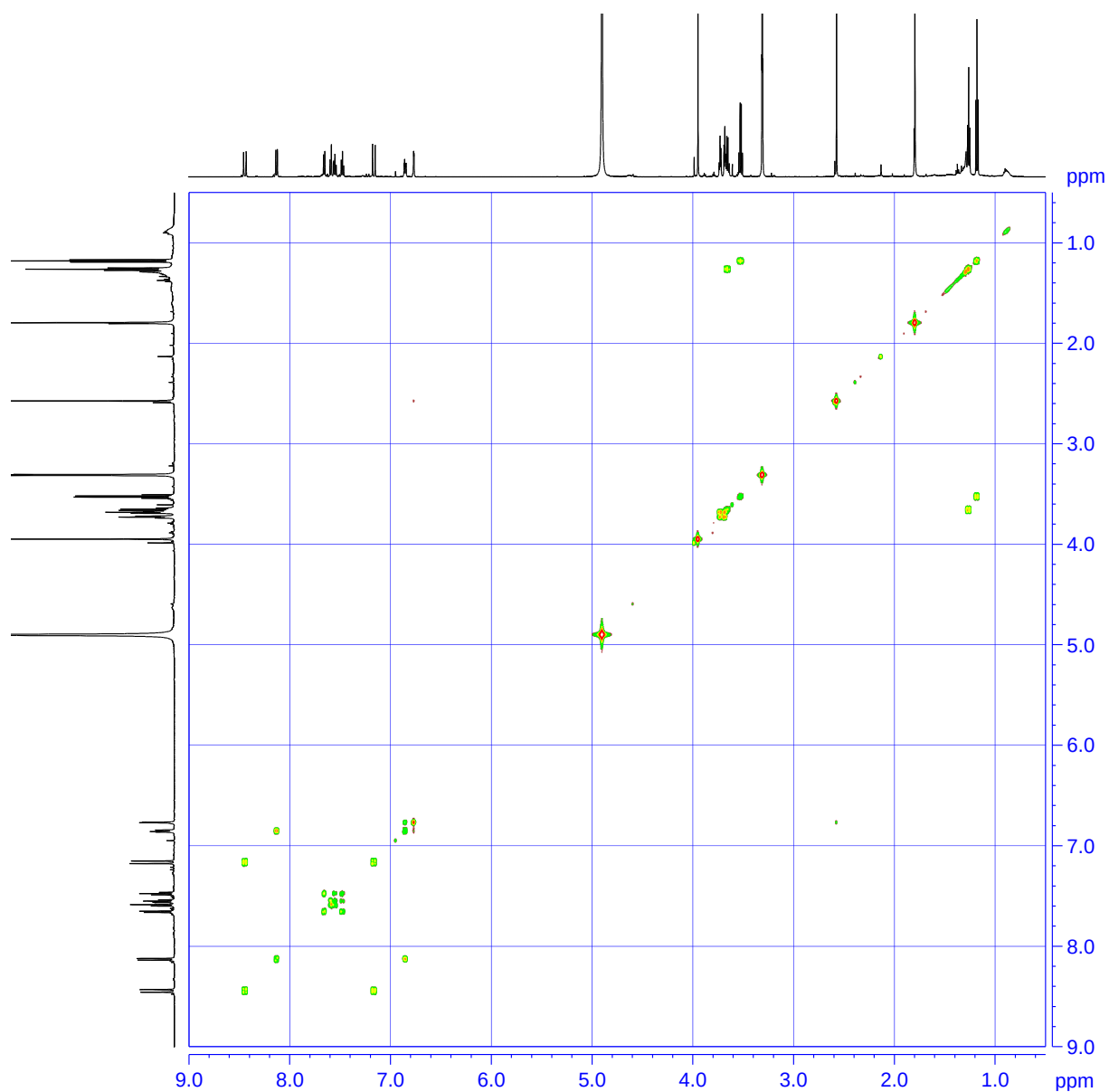


Figure S5: COSY spectrum (600 MHz, CD₃OD) of UnkV

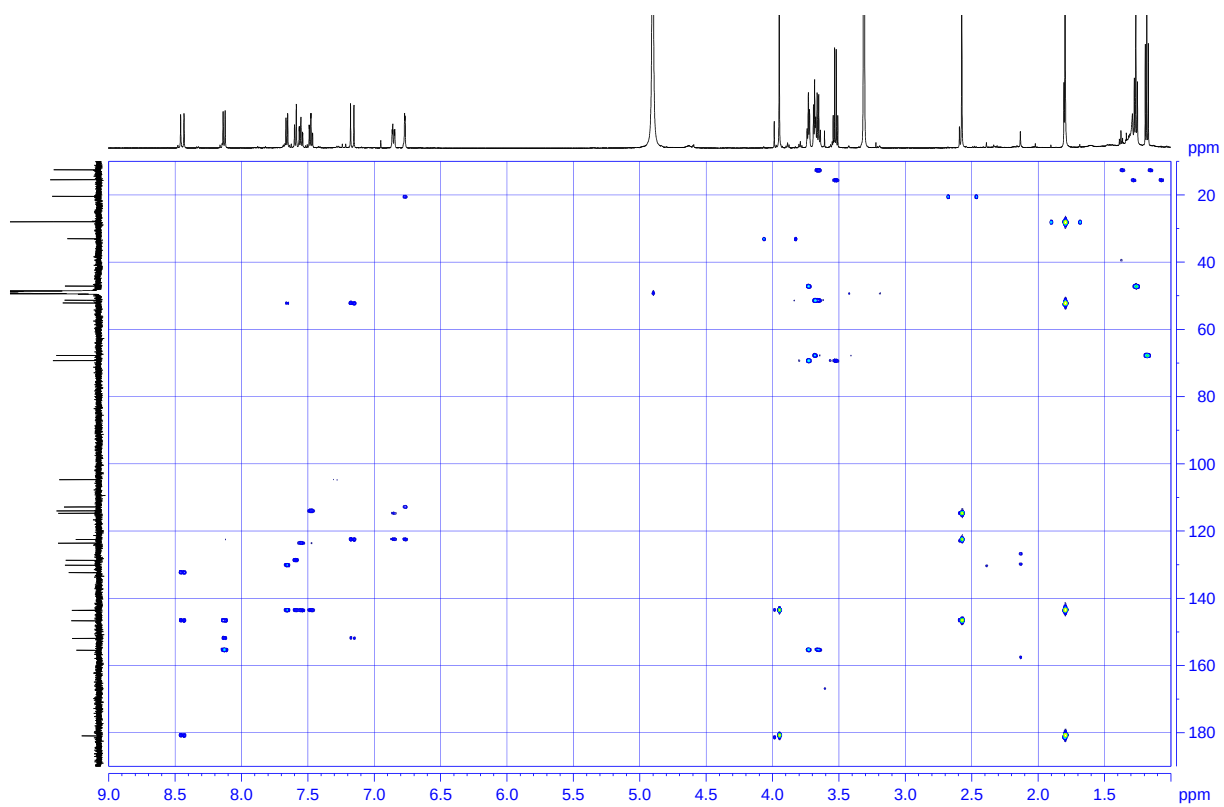


Figure S6: HMBC spectrum (600 MHz, CD₃OD) of UnkV

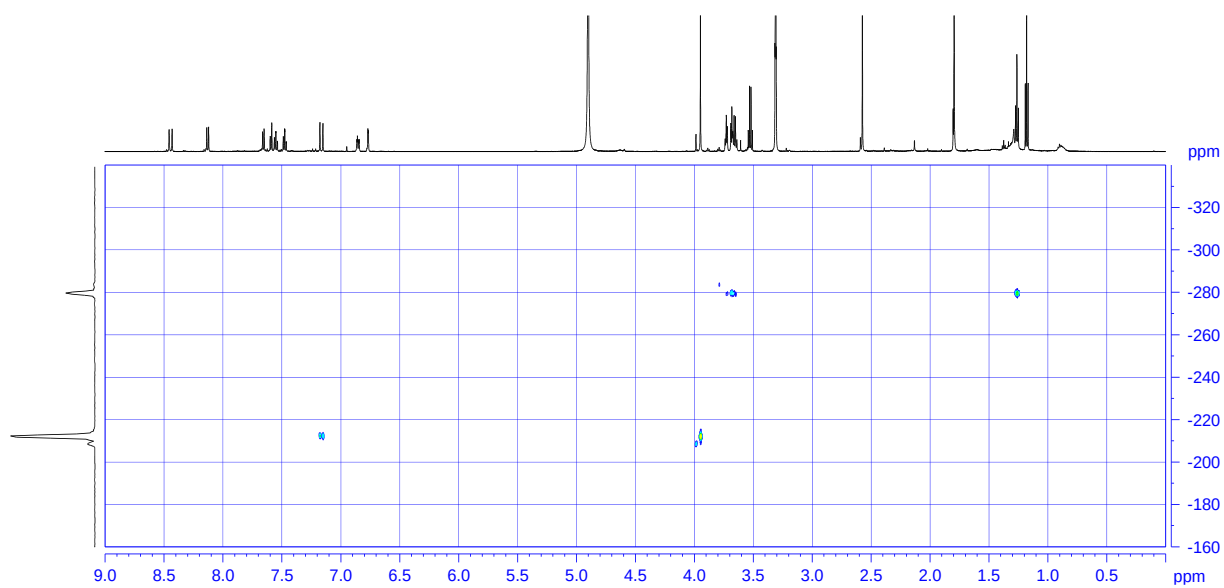


Figure S7: ¹H/¹⁵N-HMBC spectrum of UnkV

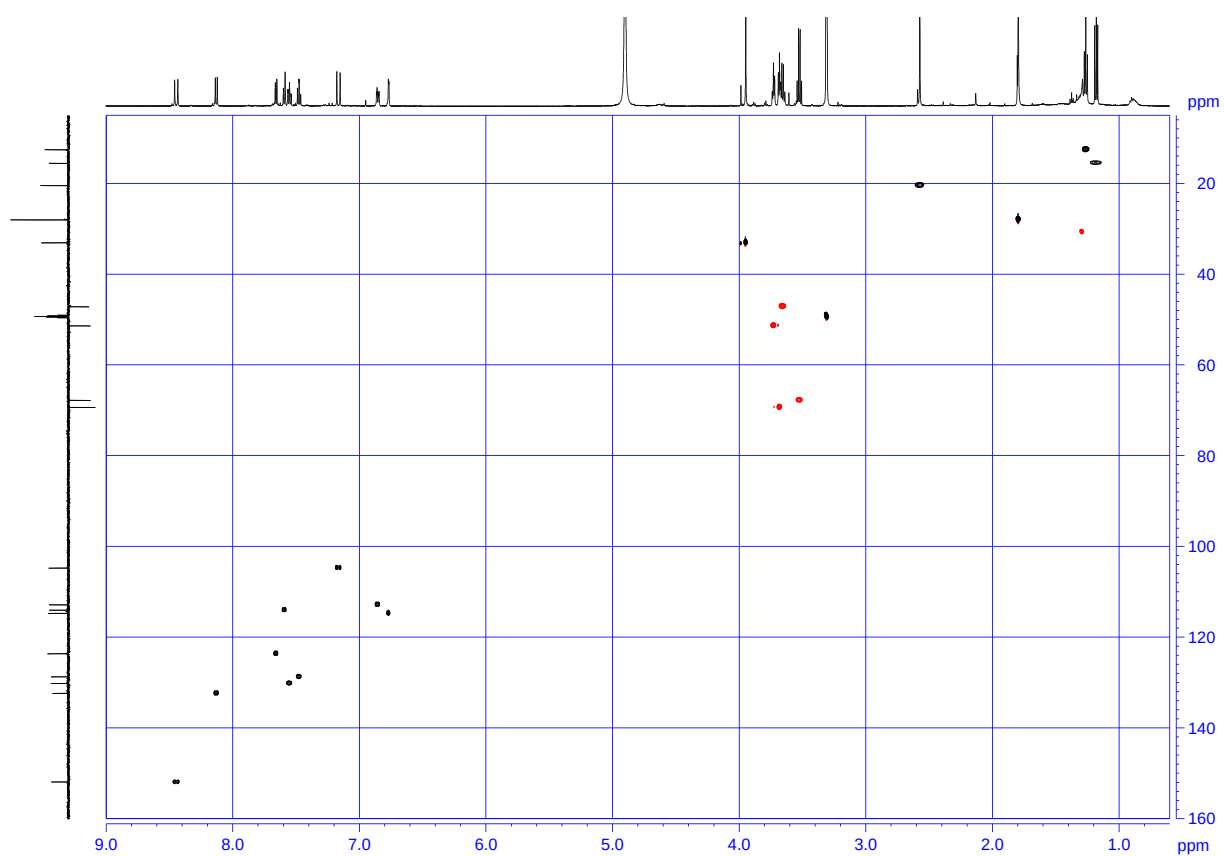


Figure S8: HSQC spectrum (600 MHz, CD_3OD) of UnkV (multiplicity edited, CH_3 and CH black, CH_2 red)

Table S2: Summary of the degradation products found with HPLC–HR-MS/MS

Origin	Exact Mass	Molecular Formula	Minor (+)/Major (++)	Degradation Type
Rh6G*	443.2329	$C_{28}H_{31}N_2O_3^+$		Starting substance
	415.2016	$C_{26}H_{27}N_2O_3^+$	+	N-deethylation
	387.1703	$C_{24}H_{23}N_2O_3^+$	+	N-deethylation
BR1:1	429.2173	$C_{27}H_{29}N_2O_3^+$		Starting substance
	415.2016	$C_{26}H_{27}N_2O_3^+$	+	Dealkylation/impurity
	401.1860	$C_{25}H_{25}N_2O_3^+$	++	N-deethylation
	387.1703	$C_{24}H_{23}N_2O_3^+$	+	Dealkylation/impurity
	373.1547	$C_{23}H_{21}N_2O_3^+$	++	N-deethylation
	359.1390	$C_{22}H_{19}N_2O_3^+$	+	Dealkylation/impurity
	445.2122	$C_{27}H_{29}N_2O_4^+$	+	Hydroxylation
	431.1965	$C_{26}H_{27}N_2O_4^+$	+	Hydroxylation/dealkylation
	417.1809	$C_{25}H_{25}N_2O_4^+$	+	Hydroxylation/N-deethylation
	403.1652	$C_{24}H_{23}N_2O_4^+$	+	Hydroxylation/dealkylation
	389.1496	$C_{23}H_{21}N_2O_4^+$	+	Hydroxylation/N-deethylation
	443.1965	$C_{27}H_{27}N_2O_4^+$	++	Oxidation
	429.1809	$C_{26}H_{25}N_2O_4^+$	+	Oxidation/dealkylation
	415.1652	$C_{25}H_{23}N_2O_4^+$	++	Oxidation/N-deethylation
	401.1495	$C_{24}H_{21}N_2O_4^+$	++	Oxidation/dealkylation
	387.1339	$C_{23}H_{19}N_2O_4^+$	++	Oxidation/N-deethylation
	373.1183	$C_{22}H_{17}N_2O_4^+$	+	Oxidation/dealkylation
	459.1914	$C_{27}H_{27}N_2O_5^+$	+	Oxidation
	431.1601	$C_{25}H_{23}N_2O_5^+$	+	Oxidation/N-deethylation
	417.1445	$C_{24}H_{21}N_2O_5^+$	+	Oxidation/dealkylation
	403.1288	$C_{23}H_{19}N_2O_5^+$	++	Oxidation/N-deethylation
	475.1864	$C_{27}H_{27}N_2O_6^+$	+	Oxidation
	447.1551	$C_{25}H_{23}N_2O_6^+$	+	Oxidation/N-deethylation
	419.1238	$C_{23}H_{19}N_2O_6^+$	+	Oxidation/N-deethylation
	473.1707	$C_{27}H_{25}N_2O_6^+$	+	Oxidation
	445.1394	$C_{25}H_{21}N_2O_6^+$	++	Oxidation/N-deethylation
	431.1238	$C_{24}H_{19}N_2O_6^+$	+	Oxidation/dealkylation
	417.1081	$C_{23}H_{17}N_2O_6^+$	++	Oxidation/N-deethylation
Rh575	415.2016	$C_{26}H_{27}N_2O_3^+$		Starting substance
	401.1860	$C_{25}H_{25}N_2O_3^+$	+	Dealkylation/impurity
	387.1703	$C_{24}H_{23}N_2O_3^+$	++	N-deethylation
	359.1390	$C_{22}H_{19}N_2O_3^+$	++	N-deethylation
	431.1965	$C_{26}H_{27}N_2O_4^+$	++	Hydroxylation
	403.1652	$C_{24}H_{23}N_2O_4^+$	+	Hydroxylation/N-deethylation
	375.1339	$C_{22}H_{19}N_2O_4^+$	+	Hydroxylation/N-deethylation
	401.1496	$C_{24}H_{21}N_2O_4^+$	+	Oxidation/N-deethylation
	387.1339	$C_{23}H_{19}N_2O_4^+$	+	Oxidation/N-deethylation
	373.1183	$C_{22}H_{17}N_2O_4^+$	+	Oxidation/N-deethylation
	429.1809	$C_{26}H_{25}N_2O_4^+$	++	Oxidation
	445.1758	$C_{26}H_{25}N_2O_5^+$	++	Oxidation
	417.1445	$C_{24}H_{21}N_2O_5^+$	+	Oxidation/N-deethylation
	389.1132	$C_{22}H_{17}N_2O_5^+$	+	Oxidation/N-deethylation
	459.1551	$C_{26}H_{23}N_2O_6^+$	+	Oxidation
BV11	471.2642	$C_{30}H_{35}N_2O_3^+$		Starting substance
	457.2486	$C_{29}H_{33}N_2O_3^+$	+	Dealkylation/impurity
	443.2329	$C_{28}H_{31}N_2O_3^+$	++	N-deethylation

	429.2173	$C_{27}H_{29}N_2O_3^+$	+	Dealkylation/impurity
	415.2016	$C_{26}H_{27}N_2O_3^+$	++	N-deethylation
	401.1860	$C_{25}H_{25}N_2O_3^+$	+	Dealkylation/impurity
	387.1703	$C_{24}H_{23}N_2O_3^+$	++	N-deethylation
	373.1547	$C_{23}H_{21}N_2O_3^+$	+	Dealkylation/impurity
	359.1390	$C_{22}H_{19}N_2O_3^+$	++	N-deethylation
	345.1234	$C_{21}H_{17}N_2O_3^+$	+	Dealkylation/impurity
	331.1077	$C_{20}H_{15}N_2O_3^+$	+	Deethylation
	487.2591	$C_{30}H_{35}N_2O_4^+$	+	Hydroxylation
	459.2278	$C_{28}H_{31}N_2O_4^+$	+	Hydroxylation/N-deethylation
	445.2122	$C_{27}H_{29}N_2O_4^+$	+	Hydroxylation/dealkylation
	431.1965	$C_{26}H_{27}N_2O_4^+$	+	Hydroxylation/N-deethylation
	403.1652	$C_{24}H_{23}N_2O_4^+$	+	Hydroxylation/N-deethylation
	389.1496	$C_{23}H_{21}N_2O_4^+$	+	Hydroxylation/dealkylation
	375.1339	$C_{22}H_{19}N_2O_4^+$	+	Hydroxylation/N-deethylation
	457.2122	$C_{28}H_{29}N_2O_4^+$	++	Oxidation/N-deethylation
	443.1965	$C_{27}H_{27}N_2O_4^+$	+	Oxidation/dealkylation
	429.1809	$C_{26}H_{25}N_2O_4^+$	+	Oxidation/N-deethylation
	415.1652	$C_{25}H_{23}N_2O_4^+$	+	Oxidation/dealkylation
	401.1496	$C_{24}H_{21}N_2O_4^+$	+	Oxidation/N-deethylation
	387.1339	$C_{23}H_{19}N_2O_4^+$	+	Oxidation/dealkylation
	501.2384	$C_{30}H_{33}N_2O_5^+$	+	Oxidation
	473.2071	$C_{28}H_{29}N_2O_5^+$	+	Oxidation/N-deethylation
	443.1601	$C_{26}H_{23}N_2O_5^+$	+	Oxidation/N-deethylation
BV11:1	457.2486	$C_{29}H_{33}N_2O_3^+$		Starting substance
	471.2642	$C_{30}H_{35}N_2O_3^+$	++	Impurity
	443.2329	$C_{28}H_{31}N_2O_3^+$	+	Dealkylation/impurity
	429.2173	$C_{27}H_{29}N_2O_3^+$	++	N-deethylation
	415.2016	$C_{26}H_{27}N_2O_3^+$	+	Dealkylation/impurity
	401.1860	$C_{25}H_{25}N_2O_3^+$	++	N-deethylation
	387.1703	$C_{24}H_{23}N_2O_3^+$	+	Dealkylation/impurity
	373.1547	$C_{23}H_{21}N_2O_3^+$	++	N-deethylation
	359.1390	$C_{22}H_{19}N_2O_3^+$	+	Dealkylation/impurity
	345.1234	$C_{21}H_{17}N_2O_3^+$	++	N-deethylation
	331.1077	$C_{20}H_{15}N_2O_3^+$	+	Dealkylation/impurity
	473.2435	$C_{29}H_{33}N_2O_4^+$	++	Hydroxylation
	459.2278	$C_{28}H_{31}N_2O_4^+$	+	Hydroxylation/dealkylation
	445.2122	$C_{27}H_{29}N_2O_4^+$	+	Hydroxylation/N-deethylation
	431.1965	$C_{26}H_{27}N_2O_4^+$	+	Hydroxylation/dealkylation
	417.1809	$C_{25}H_{25}N_2O_4^+$	+	Hydroxylation/N-deethylation
	403.1652	$C_{24}H_{23}N_2O_4^+$	+	Hydroxylation/dealkylation
	389.1496	$C_{23}H_{21}N_2O_4^+$	+	Hydroxylation/N-deethylation
	375.1339	$C_{22}H_{19}N_2O_4^+$	+	Hydroxylation/dealkylation
	361.1183	$C_{21}H_{17}N_2O_4^+$	+	Hydroxylation/N-deethylation
	471.2278	$C_{29}H_{31}N_2O_4^+$	++	Oxidation
	457.2122	$C_{28}H_{29}N_2O_4^+$	+	Oxidation/dealkylation
	443.1965	$C_{27}H_{27}N_2O_4^+$	++	Oxidation/N-deethylation
	429.1809	$C_{26}H_{25}N_2O_4^+$	+	Oxidation/dealkylation
	415.1652	$C_{25}H_{23}N_2O_4^+$	++	Oxidation/N-deethylation
	401.1496	$C_{24}H_{21}N_2O_4^+$	+	Oxidation/dealkylation
	387.1339	$C_{23}H_{19}N_2O_4^+$	++	Oxidation/N-deethylation

	373.1183	$C_{22}H_{17}N_2O_4^+$	+	Oxidation/dealkylation
	459.2642	$C_{29}H_{35}N_2O_3^+$	++	Reduction
	417.2173	$C_{26}H_{29}N_2O_3^+$	+	Dealkylation/reduction
	459.1914	$C_{27}H_{27}N_2O_5^+$	+	Oxidation/N-deethylation
	487.2227	$C_{29}H_{31}N_2O_5^+$	+	Oxidation
	431.1601	$C_{25}H_{23}N_2O_5^+$	+	Oxidation/N-deethylation
RhB	443.2329	$C_{28}H_{31}N_2O_3^+$		Starting substance
	429.2173	$C_{27}H_{29}N_2O_3^+$	+	Dealkylation/impurity
	415.2016	$C_{26}H_{27}N_2O_3^+$	++	N-deethylation
	401.1860	$C_{25}H_{25}N_2O_3^+$	+	Dealkylation
	387.1703	$C_{24}H_{23}N_2O_3^+$	++	N-deethylation
	359.1390	$C_{22}H_{19}N_2O_3^+$	++	N-deethylation
	345.1234	$C_{21}H_{17}N_2O_3^+$	+	Dealkylation
	331.1077	$C_{20}H_{15}N_2O_3^+$	++	N-deethylation
	459.2278	$C_{28}H_{31}N_2O_4^+$	++	Hydroxylation
	431.1965	$C_{26}H_{27}N_2O_4^+$	++	Hydroxylation/N-deethylation
	403.1652	$C_{24}H_{23}N_2O_4^+$	++	Hydroxylation/N-deethylation
	375.1339	$C_{22}H_{19}N_2O_4^+$	+	Hydroxylation/N-deethylation
	347.1026	$C_{20}H_{15}N_2O_4^+$	+	Hydroxylation/N-deethylation
	445.2486	$C_{28}H_{33}N_2O_3^+$	+	Reduction
	461.2435	$C_{28}H_{33}N_2O_4^+$	+	Hydroxylation/reduction
	473.2071	$C_{28}H_{29}N_2O_5^+$	+	Oxidation
	445.1758	$C_{26}H_{25}N_2O_5^+$	+	Oxidation/N-deethylation
	417.2173	$C_{26}H_{29}N_2O_3^+$	+	N-deethylation/reduction
SRB	559.1567	$C_{27}H_{31}N_2O_7S_2^+$		Starting substance
	531.1254	$C_{25}H_{27}N_2O_7S_2^+$	++	N-deethylation
	503.0941	$C_{23}H_{23}N_2O_7S_2^+$	+	N-deethylation
	475.0628	$C_{21}H_{19}N_2O_7S_2^+$	+	N-deethylation
	447.0315	$C_{19}H_{15}N_2O_7S_2^+$	+	N-deethylation
	575.1516	$C_{27}H_{31}N_2O_8S_2^+$	+	Hydroxylation
SY172	414.1118	$C_{20}H_{20}N_3O_5S^+$		Starting substance
	386.0805	$C_{18}H_{16}N_3O_5S^+$	+	N-deethylation
	358.0492	$C_{16}H_{12}N_3O_5S^+$	+	N-deethylation
SY44	317.1285	$C_{20}H_{17}N_2O_2^+$		Starting substance
	302.1176	$C_{20}H_{16}NO_2^+$	+	Nitrogen elimination
	333.1234	$C_{20}H_{17}N_2O_3^+$	+	Hydroxylation
BY40	362.1863	$C_{22}H_{24}N_3O_2^+$		Starting substance
	348.1707	$C_{21}H_{22}N_3O_2^+$	+	Dealkylation
	334.1550	$C_{20}H_{20}N_3O_2^+$	++	N-deethylation
	320.1394	$C_{19}H_{18}N_3O_2^+$	+	Dealkylation
	306.1237	$C_{18}H_{16}N_3O_2^+$	++	N-deethylation
	292.1081	$C_{17}H_{14}N_3O_2^+$	+	Dealkylation
	378.1812	$C_{22}H_{24}N_3O_3^+$	++	Hydroxylation
	350.1499	$C_{20}H_{20}N_3O_3^+$	+	Hydroxylation/N-deethylation
	336.1343	$C_{19}H_{18}N_3O_3^+$	+	Hydroxylation/dealkylation
	322.1186	$C_{18}H_{16}N_3O_3^+$	+	Hydroxylation/N-deethylation
	362.1499	$C_{21}H_{20}N_3O_3^+$	+	Oxidation/dealkylation
	348.1343	$C_{20}H_{18}N_3O_3^+$	++	Oxidation/N-deethylation
	334.1186	$C_{19}H_{16}N_3O_3^+$	++	Oxidation/dealkylation
	320.1030	$C_{18}H_{14}N_3O_3^+$	+	Oxidation/N-deethylation
	352.1656	$C_{20}H_{22}N_3O_3^+$	+	Hydroxylation/reduction/

				N-deethylation
	378.1448	$C_{21}H_{20}N_3O_4^+$	+	Hydroxylation/reduction/dealkylation
	364.1292	$C_{20}H_{18}N_3O_4^+$	+	Hydroxylation/reduction/N-deethylation
	406.1397	$C_{22}H_{20}N_3O_5^+$	+	Oxidation
	394.1761	$C_{22}H_{24}N_3O_4^+$	+	Oxidation
	380.1605	$C_{21}H_{22}N_3O_4^+$	+	Oxidation/dealkylation
	319.1441	$C_{20}H_{19}N_2O_2^+$	+	N-deethylation/nitrogen elimination
FB184	431.1788	$C_{26}H_{27}N_2O_2S^+$		Starting substance
FB61	232.1332	$C_{14}H_{18}NO_2^+$		Starting substance
	204.1019	$C_{12}H_{14}NO_2^+$	++	N-deethylation
	176.0706	$C_{10}H_{10}NO_2^+$	++	N-deethylation
	208.1332	$C_{12}H_{18}NO_2^+$	++	
	248.1281	$C_{14}H_{18}NO_3^+$	+	Hydroxylation
	218.0812	$C_{12}H_{12}NO_3^+$	++	Oxidation/N-deethylation
	204.0655	$C_{11}H_{10}NO_3^+$	+	Oxidation/dealkylation

*The reference substance of Rh6G dissolved poorly, did not show strong fluorescence, and was very susceptible to light aging.