Electronic Supplementary Information

Environmentally benign and diastereoselective synthesis of 2,4,5-trisubstituted-2-imidazolines

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1. Synthesis of benzaldehyde substrates

1.1. Synthesis of methyl 4-formylbenzoate

Methyl 4-formylbenzoate was prepared according to a method previously proposed in the literature[1] with slight modifications. 4-Formylbenzoic acid (2.5 g, 16.7 mmol) was dissolved in 50 mL methanol under inert atmosphere. The reaction mixture was cooled down to 0 ºC and then $SOCl_2$ (10 mL, 136 mmol) was added dropwise under stirring. The mixture was stirred at room temperature for 24 h. The reaction was terminated by evaporating the excess methanol with a rotavap. The oily residue was poured onto 500 mL cold water to provide the product as white crystals which were collected on a vacuum filter.

Yield: 87% (2.38 g)

The obtained spectra are in good agreement with literature data[1]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 8.18 (d, *J* = 7.8 Hz, 2H), 7.94 (d, *J* = 7.8 Hz, 3H), 3.95 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.8, 166.2, 139.2, 135.2, 130.3, 129.6, 52.7; IR (ATR-FTIR) ν_{max} 2963 (CH), 2888 (CH), 1721 (C=O), 1683 (C=O), 1280 (C–C(O)–O), 1106 (C–O–C) cm^{-1}.

1.2. Synthesis of 4-formyl-*N,N,N*-trimethylanilinium iodide

4-(Dimethylamino)benzaldehyde (2 g, 13.4 mmol) in acetonitrile (15 mL) was stirred under inert atmosphere in a pressure tube. Then, methyl iodide (8.2 g, 3.6 mL, 57.8 mmol) was added to the solution. The reaction mixture was stirred at 90 ºC for 72 h. Acetonitrile was evaporated and the residue was crystallized from ethyl acetate (20 mL). The product was obtained as pale yellow crystals.

Yield: 72% (442 mg)

^{1}H NMR (400 MHz, CD_3CN) δ 10.10 (s, 1H), 8.13 (d, *J* = 9.2 Hz, 2H), 8.07 (d, *J* = 9.1 Hz, 2H), 3.66 (s, 9H); ^{13}C NMR (101 MHz, CD_3CN) δ 192.1, 151.5, 138.4, 132.0, 122.4, 58.1; MS (ESI–/SQD2) m/z: 126.8 $[I]^-$, 418.0 $[M+2I]^-$; MS (ESI+/SQD2) m/z: 149.0 $[M-{\cdot}CH_3]^{\cdot+}$; HRMS (HESI+/Orbitrap) m/z: Calcd for $[M]^+$ $C_{10}H_{14}NO$: 164.1070; Found: 164.1068; D = -1.16 ppm.

2. NMR spectra

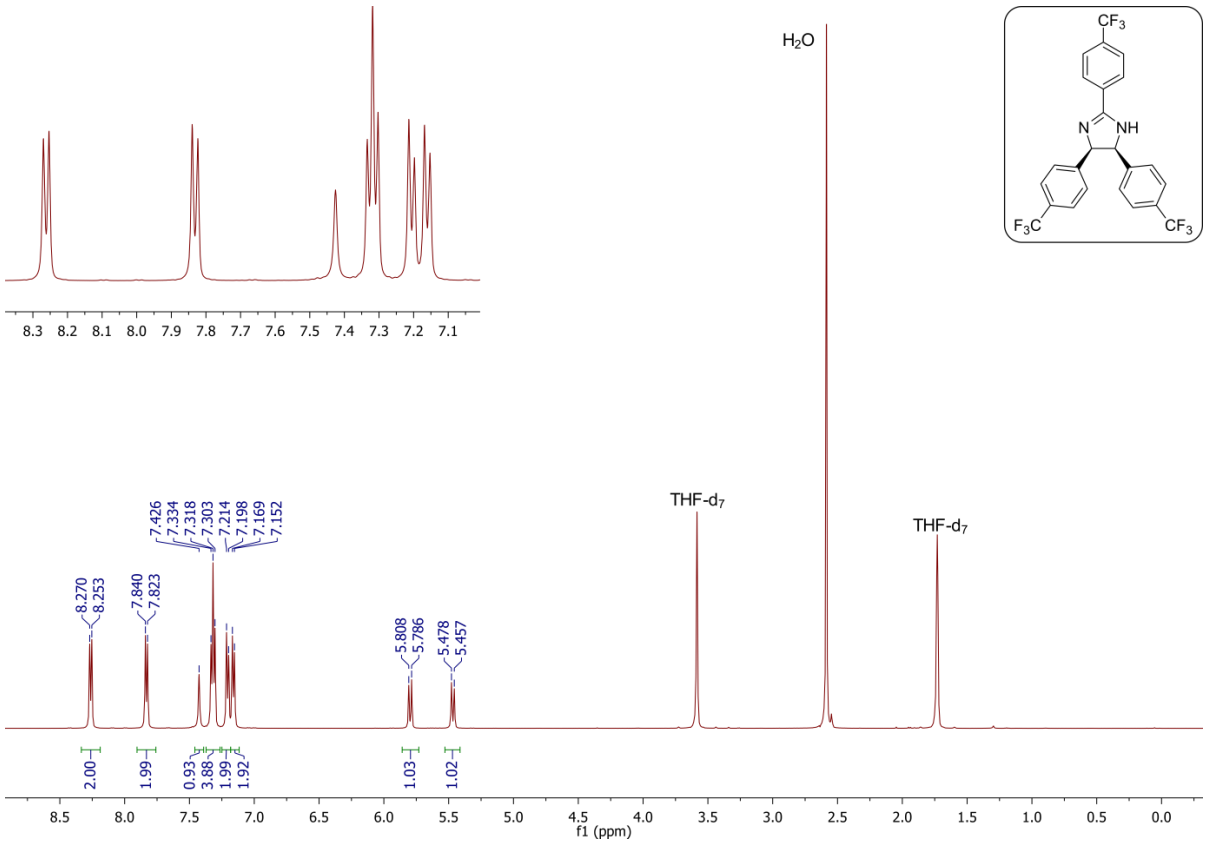


Fig. S1 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **1** with the structure in insert.

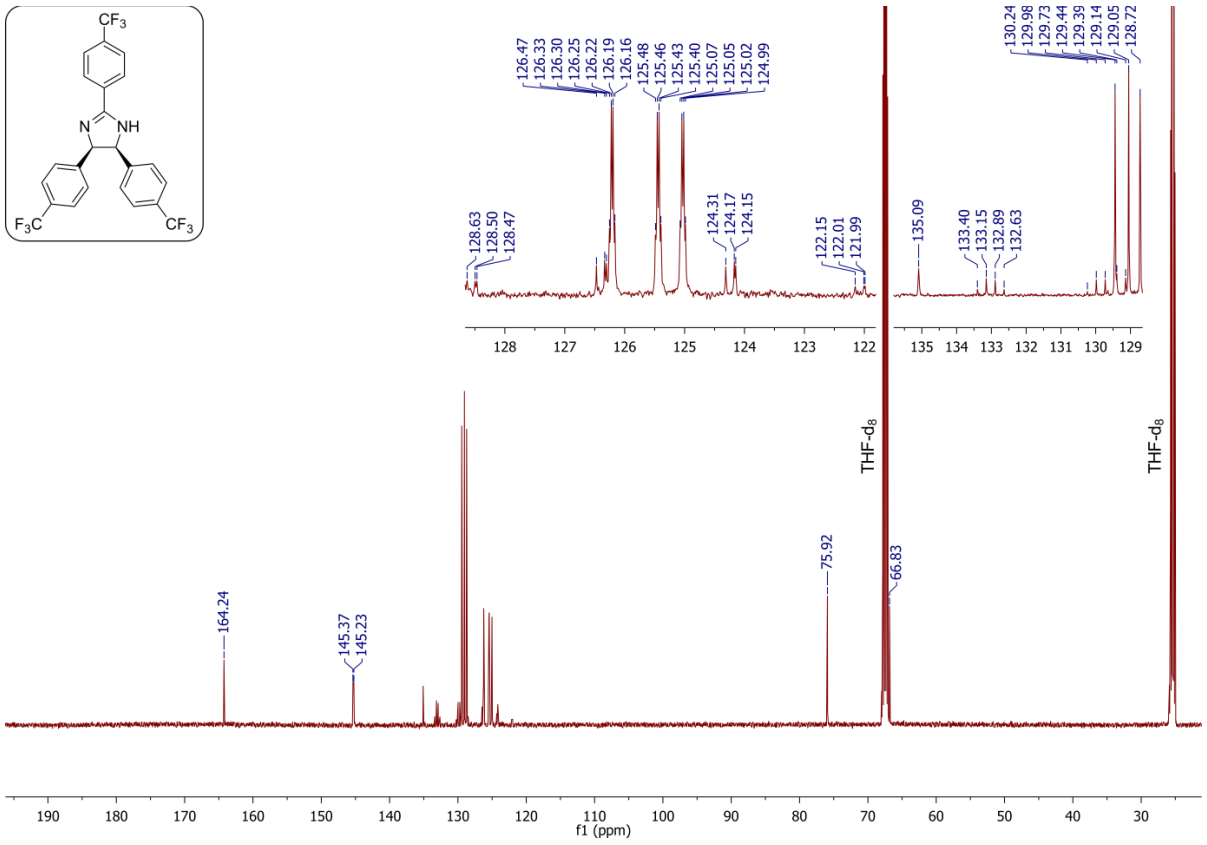


Fig. S2 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **1** with the structure in insert.

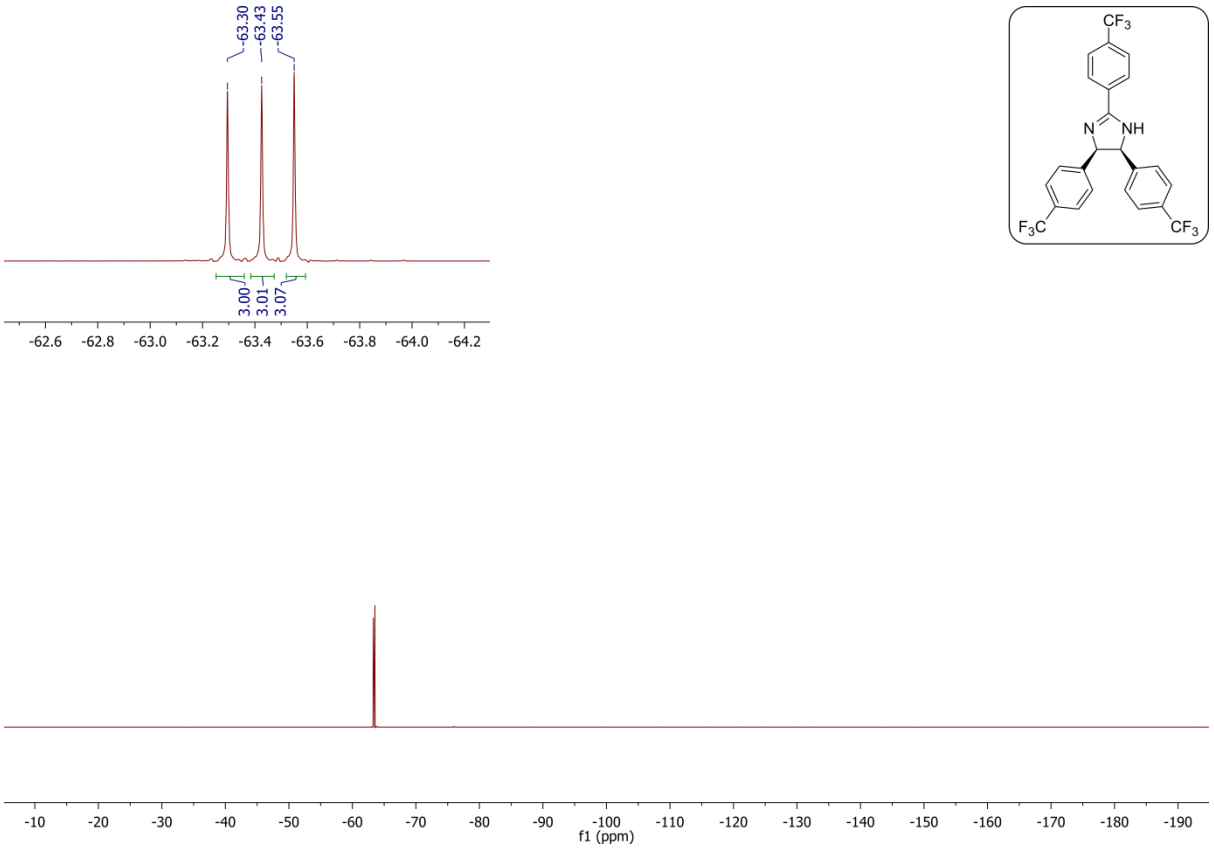


Fig. S3 ^{19}F NMR (471 MHz, THF-d_8) spectrum of **1** with the structure in insert.

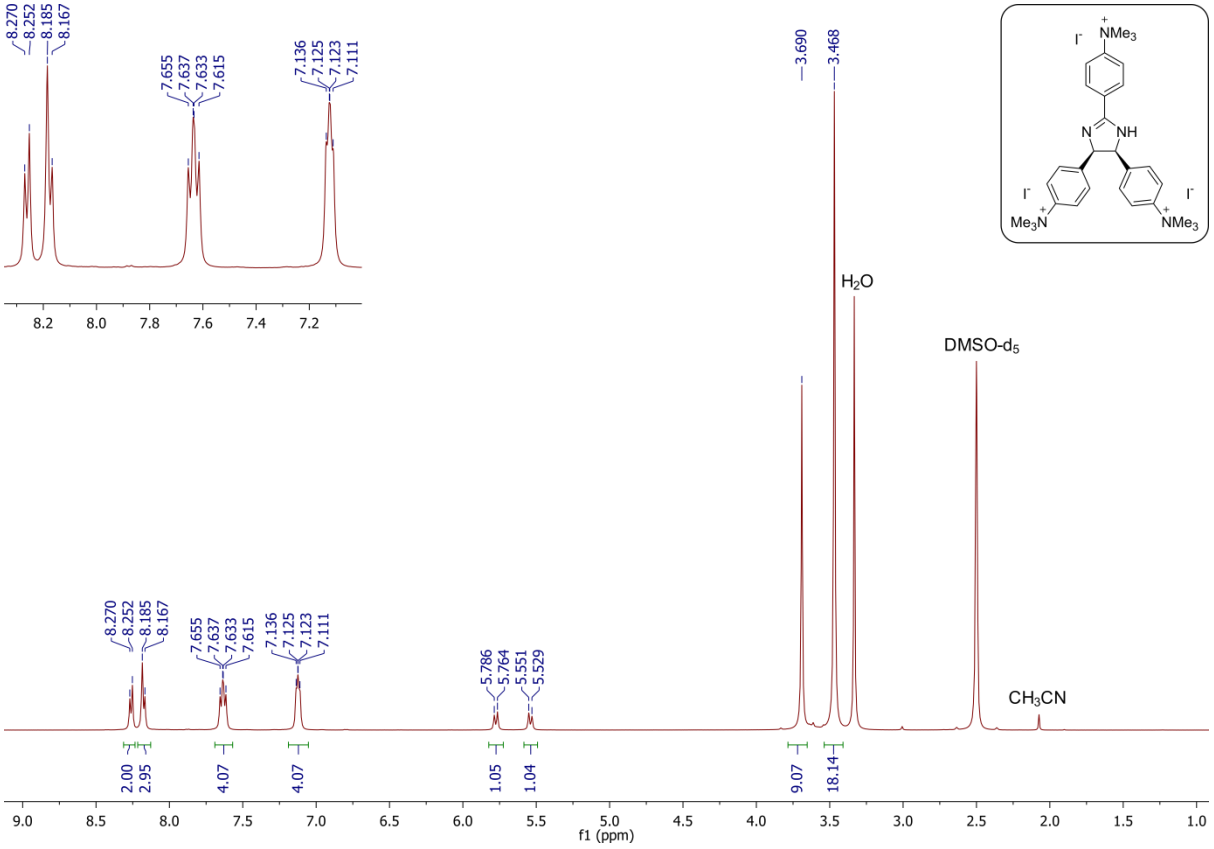


Fig. S4 ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **2** with the structure in insert.

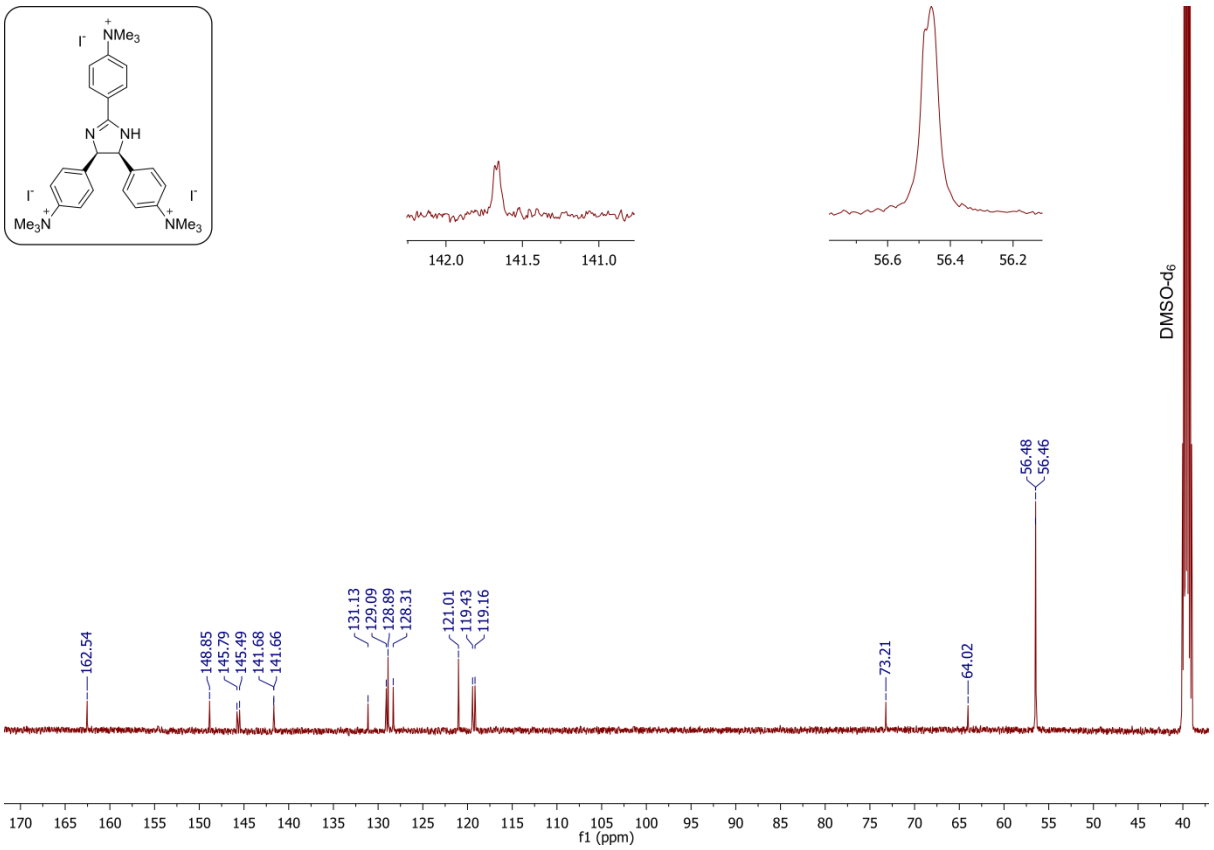


Fig. S5 ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **2** with the structure in insert.

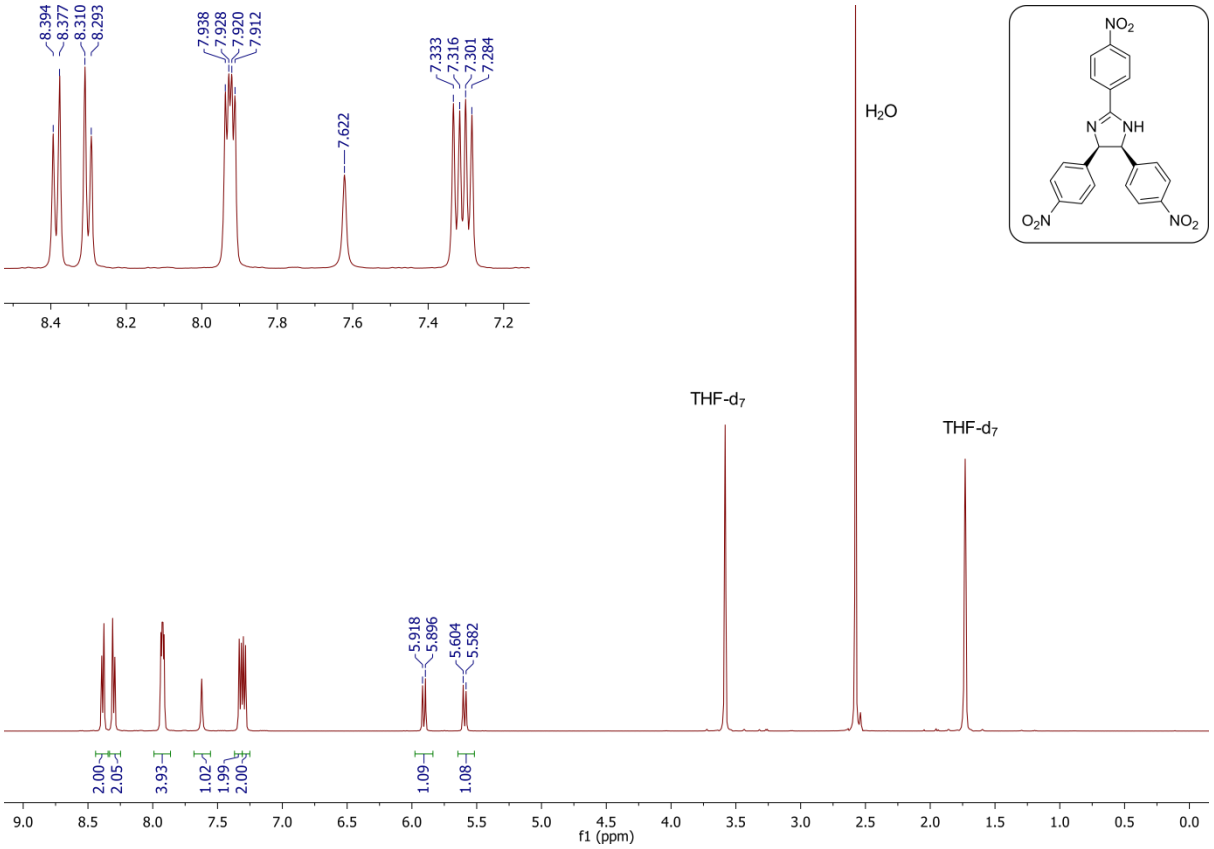


Fig. S6 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **3** with the structure in insert.

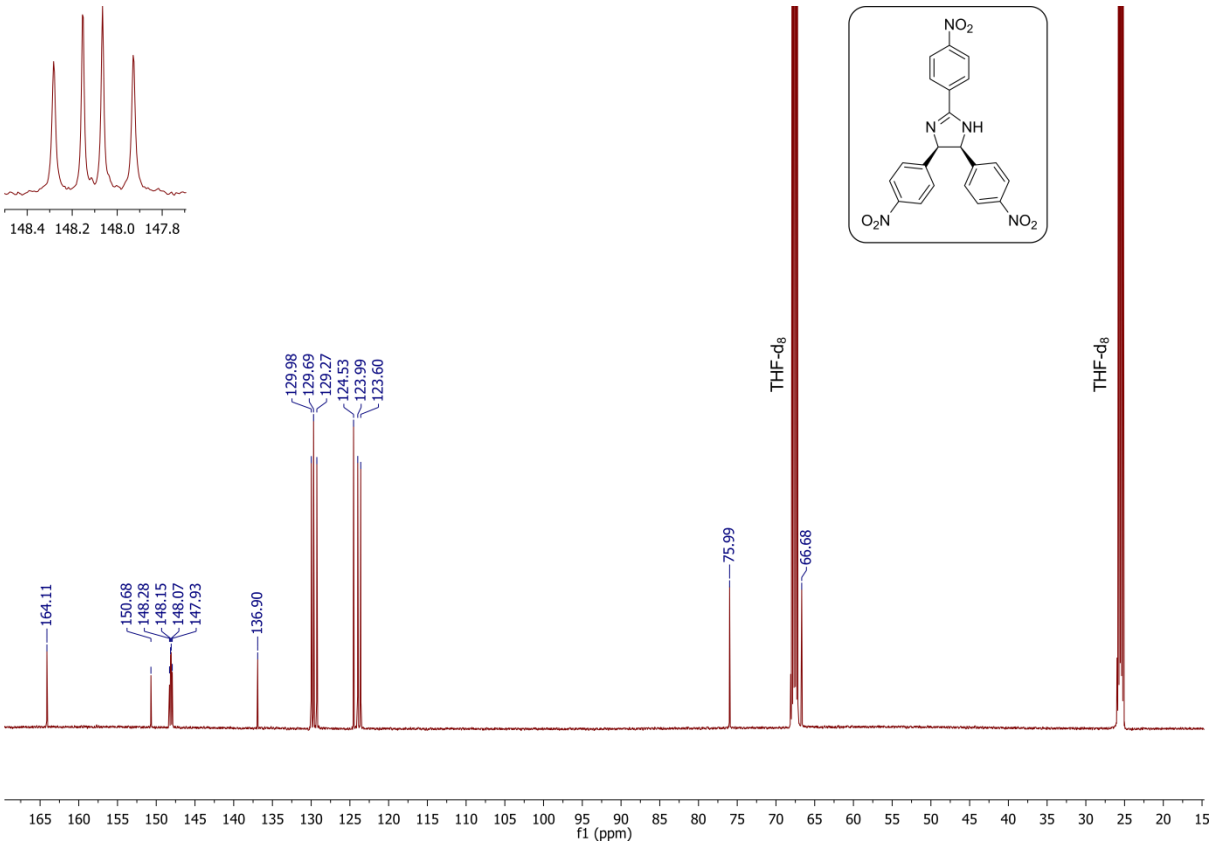


Fig. S7 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **3** with the structure in insert.

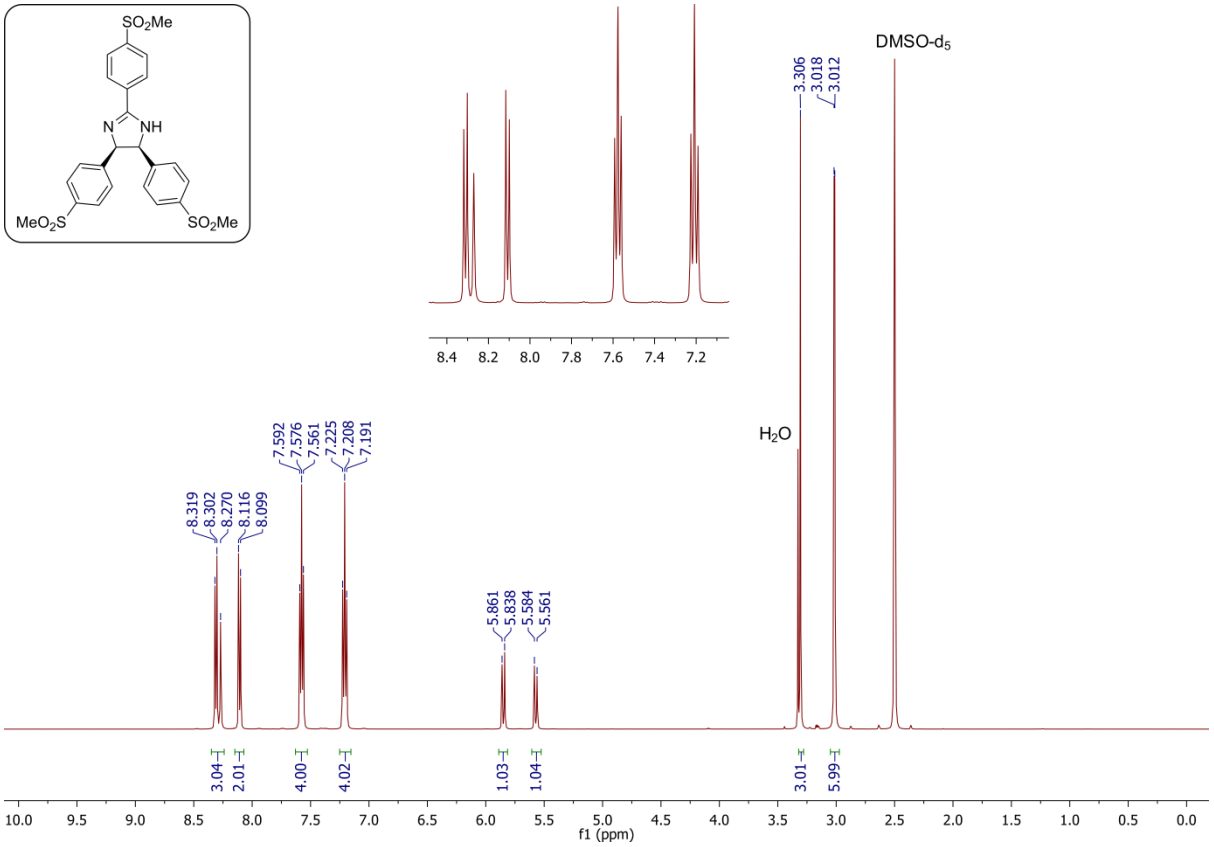


Fig. S8 ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **4** with the structure in insert.

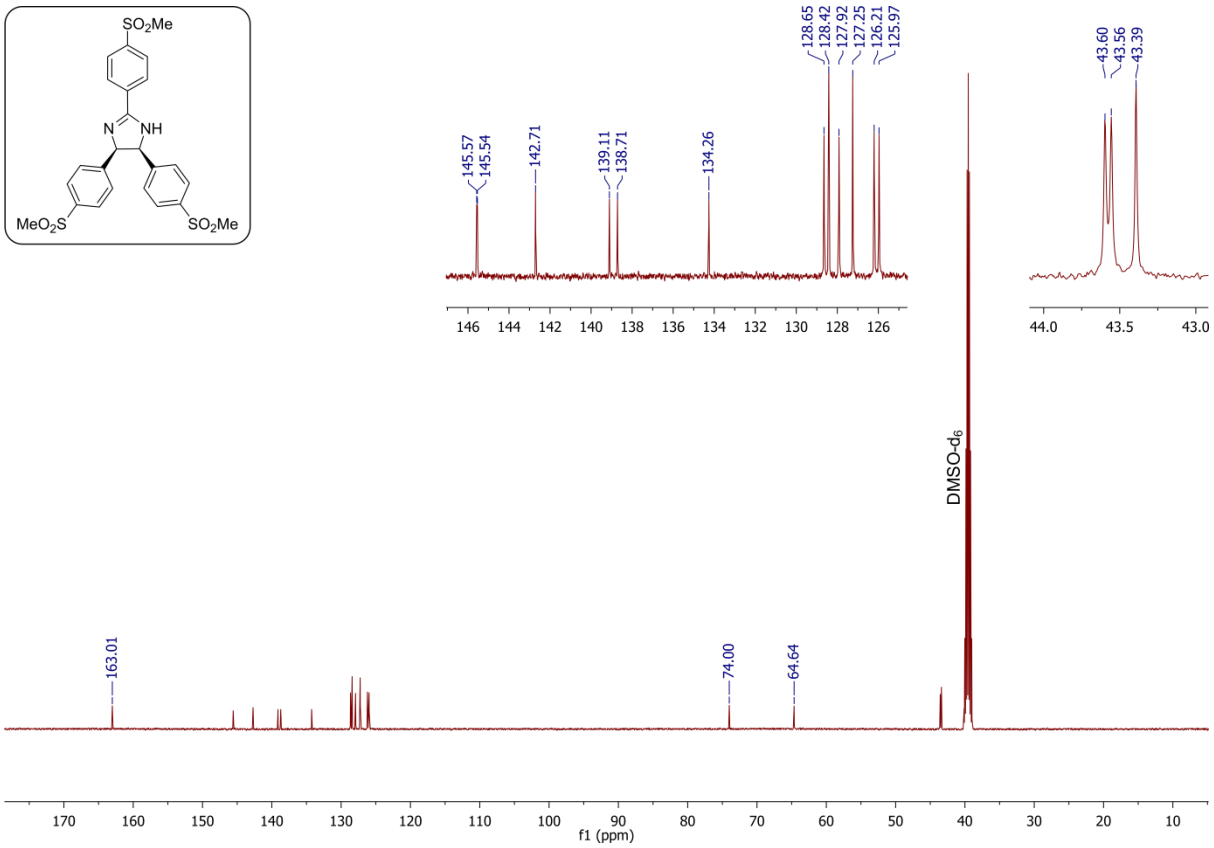


Fig. S9 ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **4** with the structure in insert.

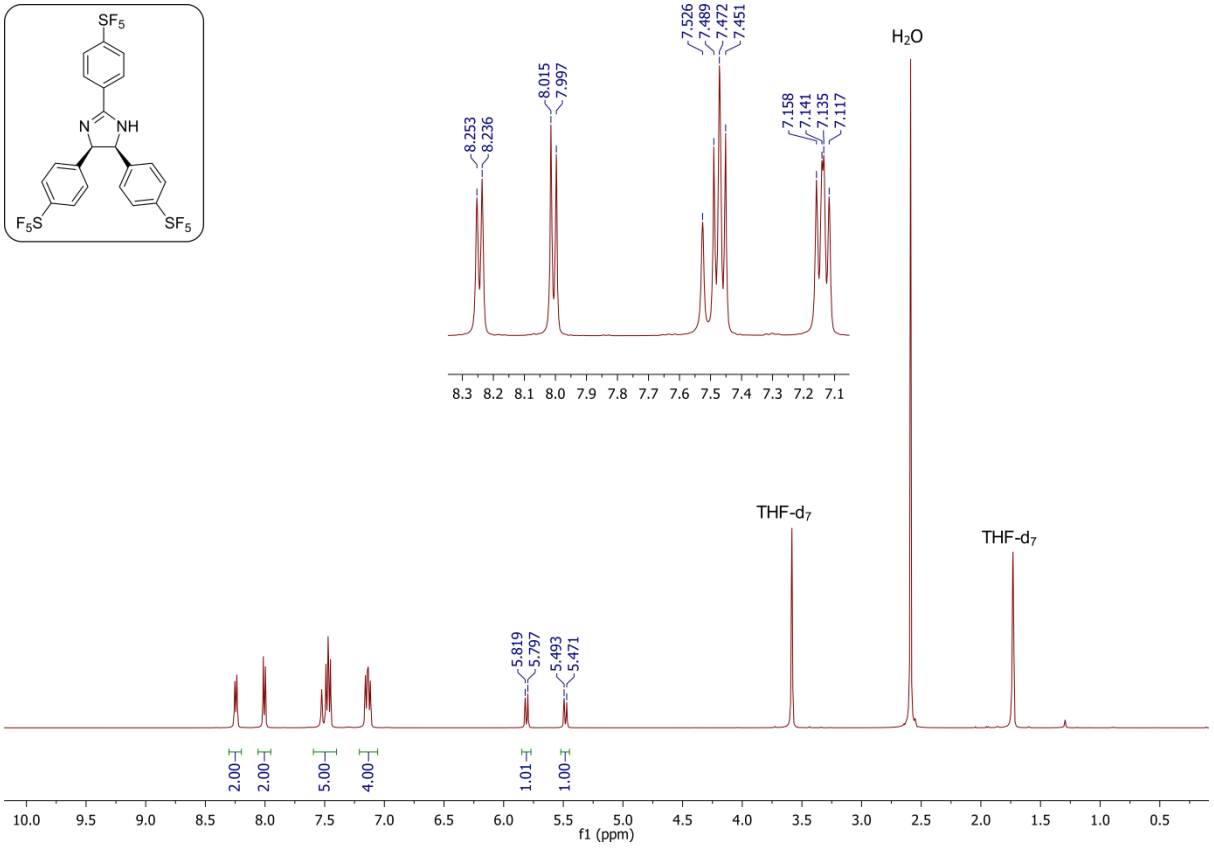


Fig. S10 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **5** with the structure in insert.

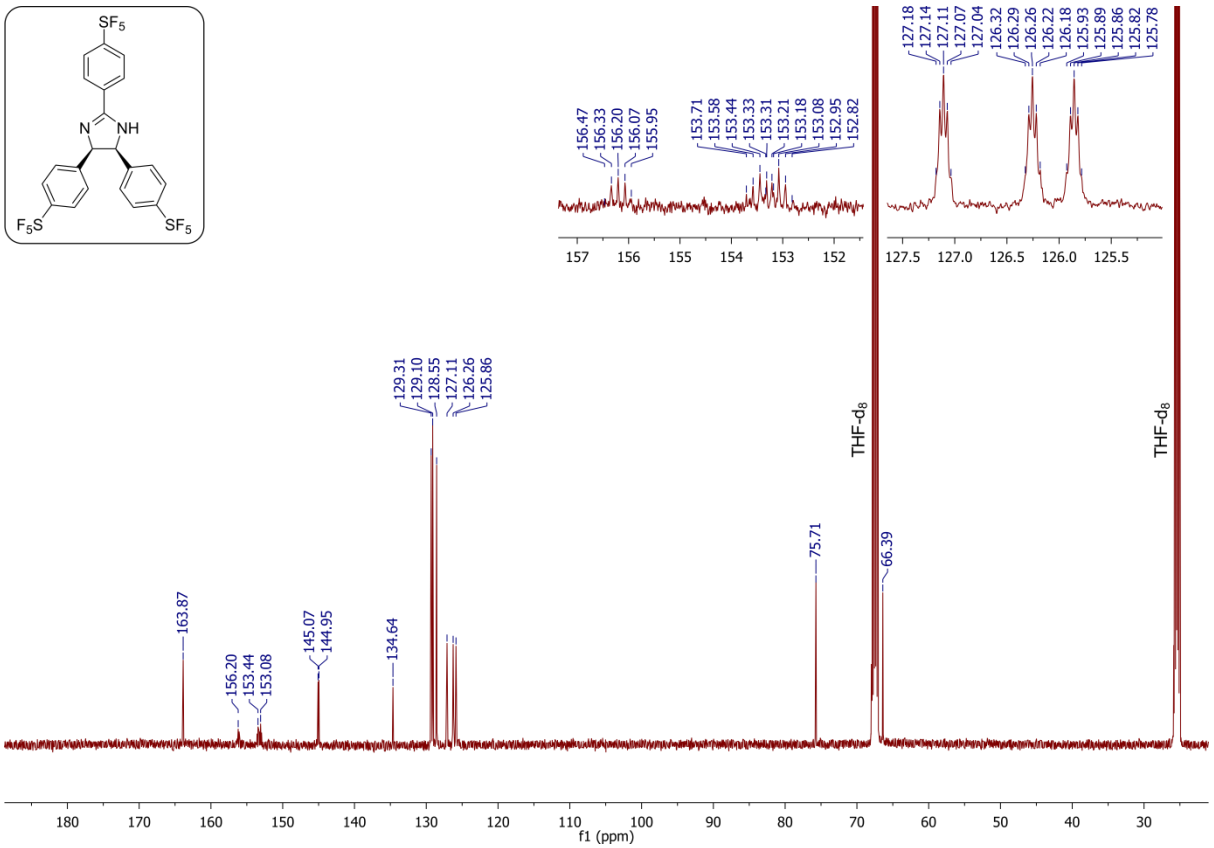


Fig. S11 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **5** with the structure in insert.

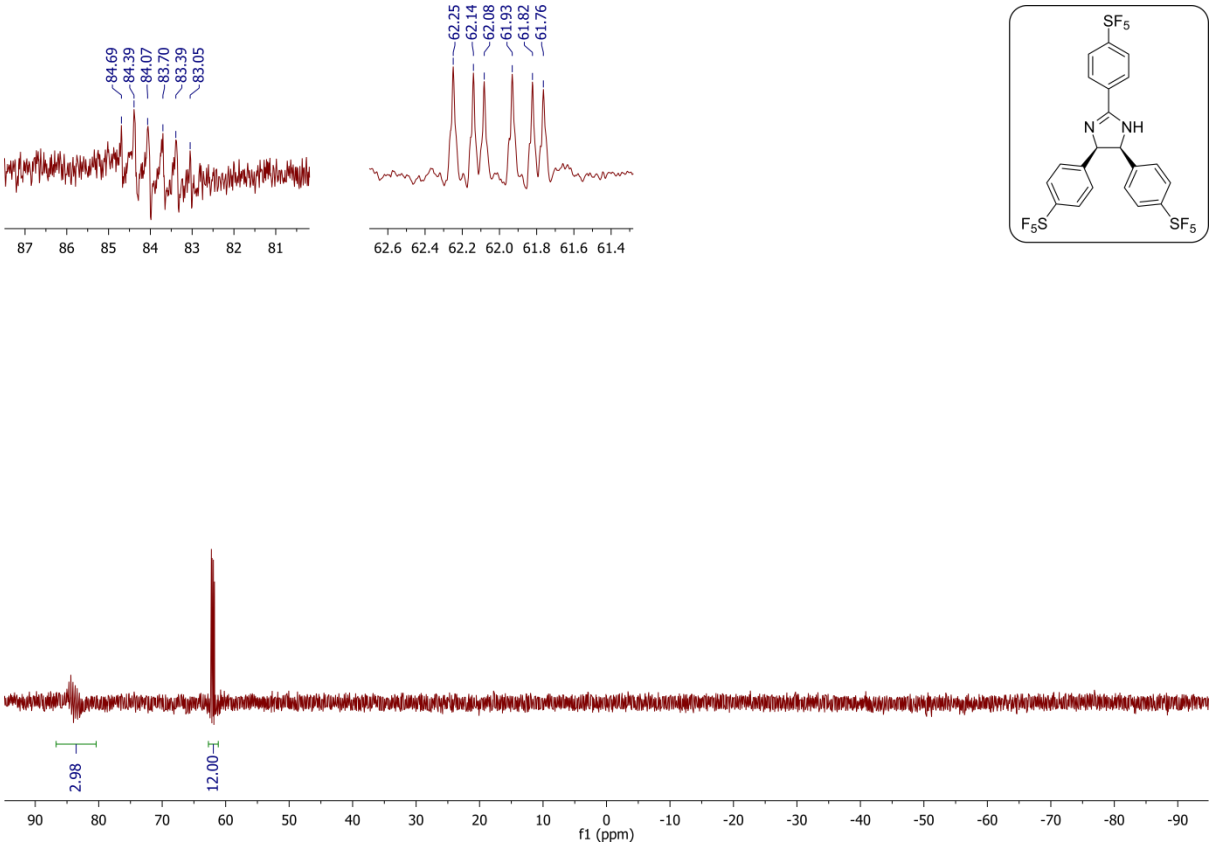


Fig. S12 ^{19}F NMR (471 MHz, THF-d_8) spectrum of **5** with the structure in insert.

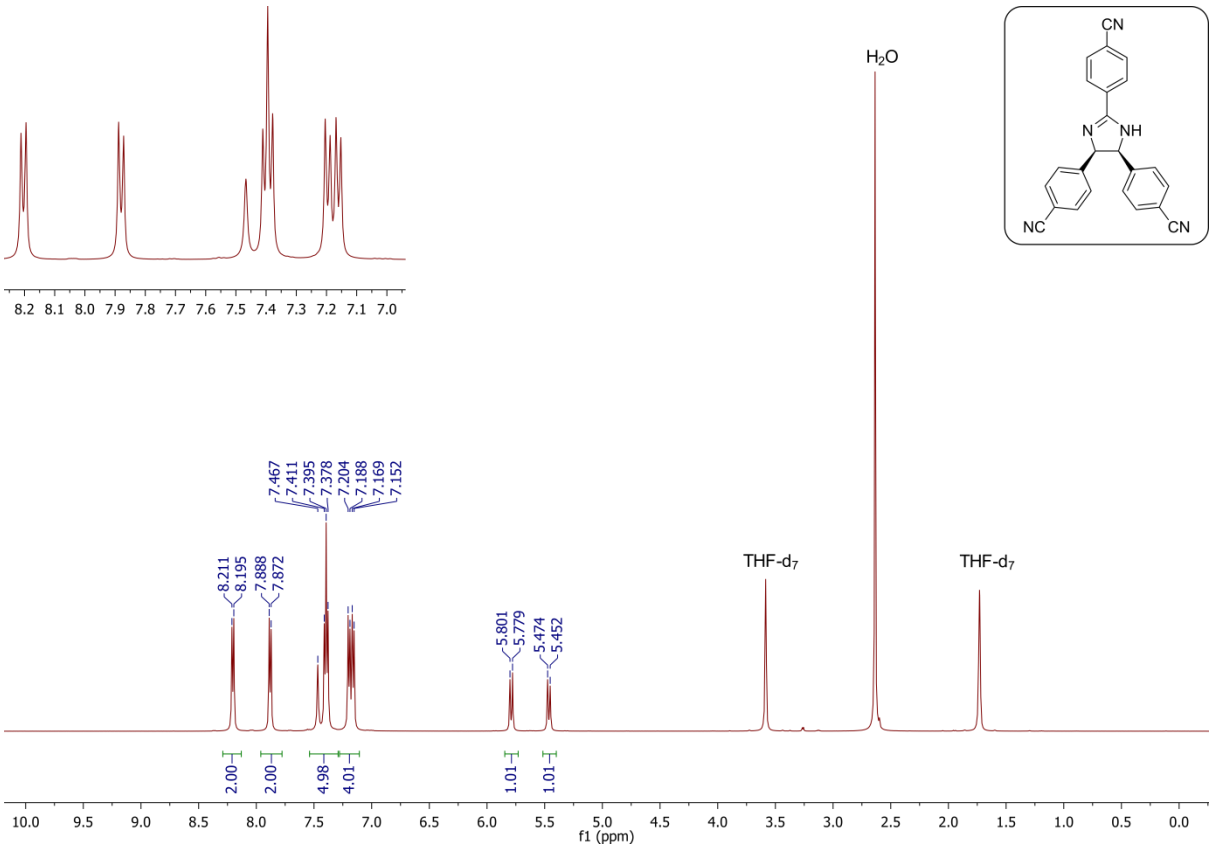


Fig. S13 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **6** with the structure in insert.

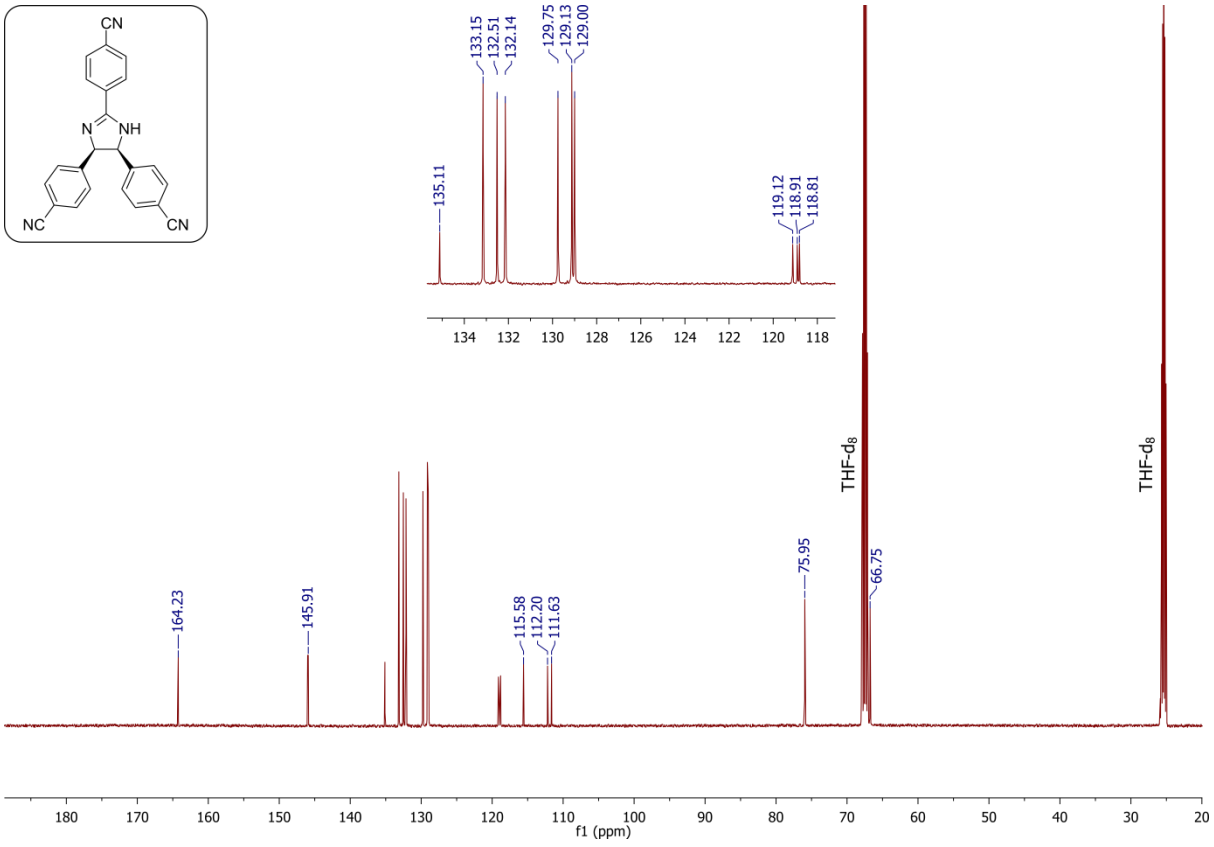


Fig. S14 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **6** with the structure in insert.

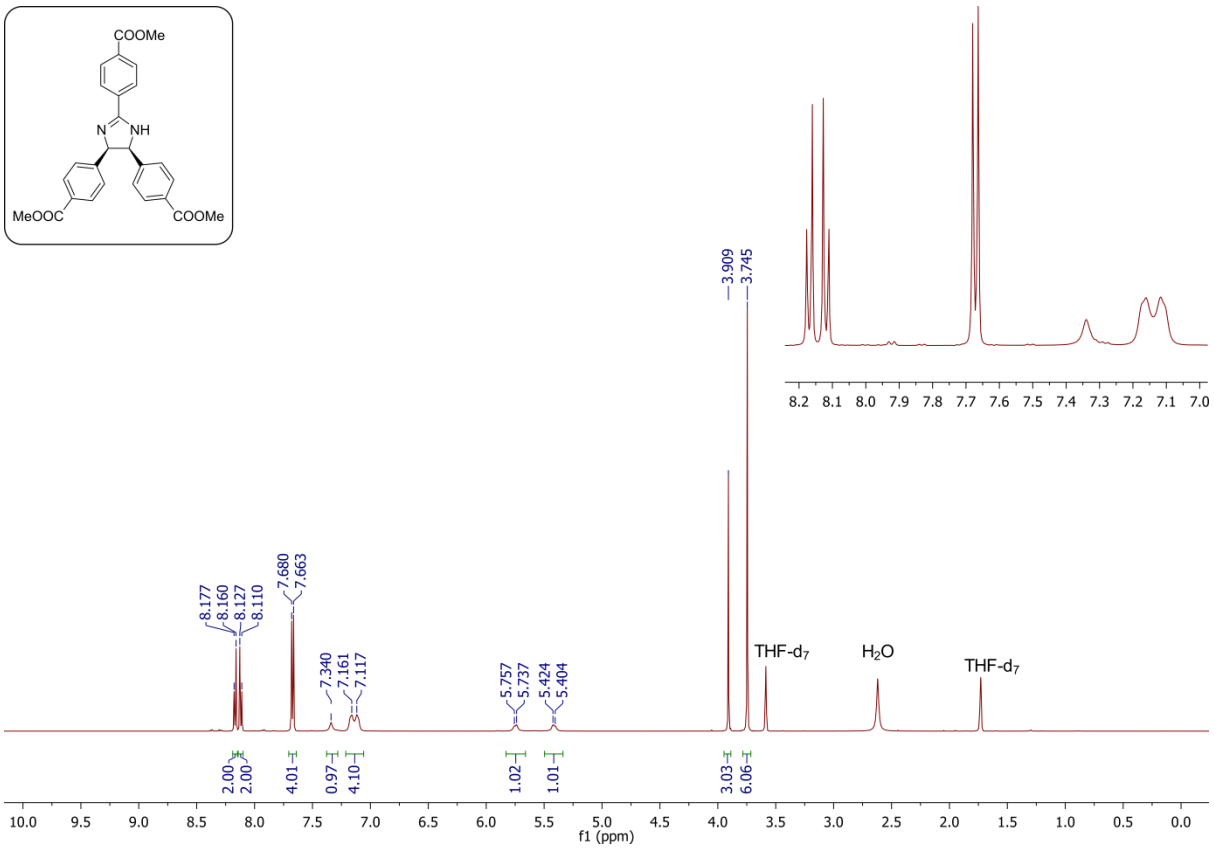


Fig. S15 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **7** with the structure in insert.

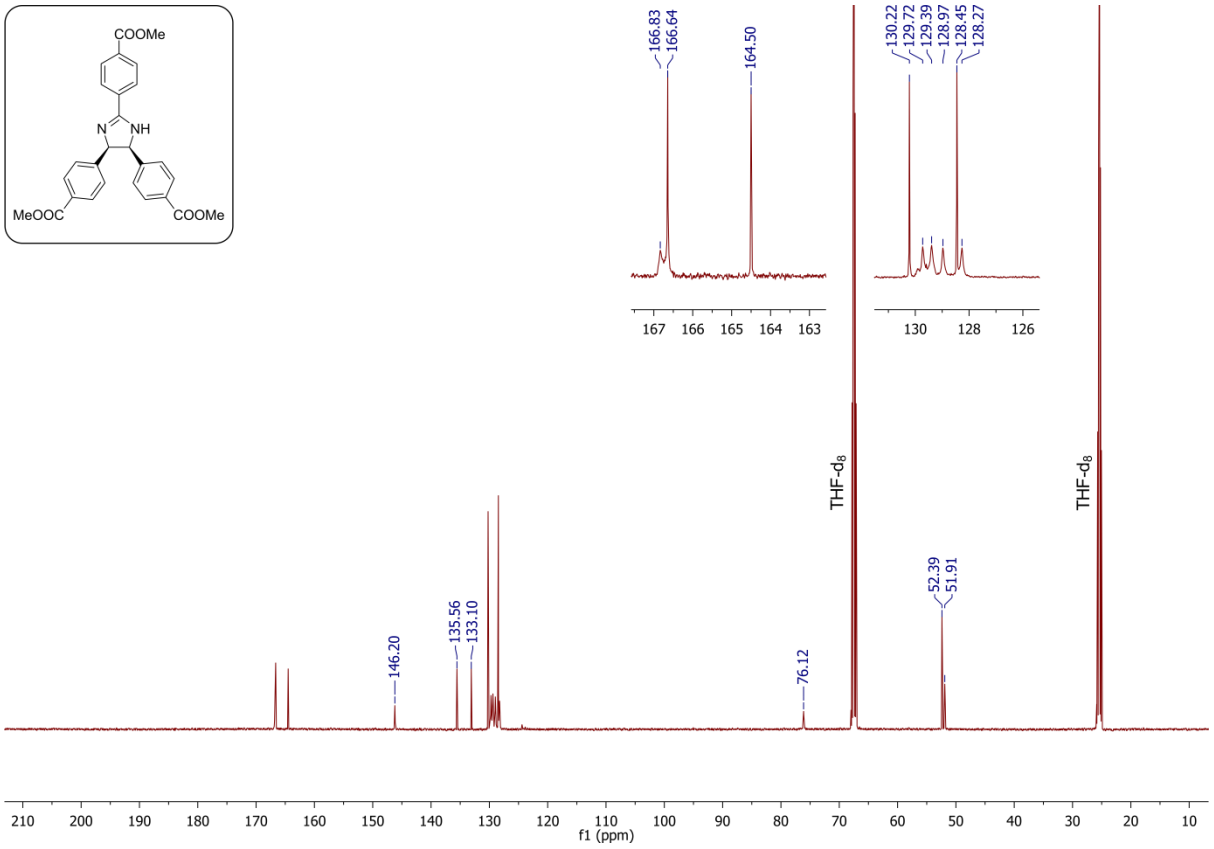


Fig. S16 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **7** with the structure in insert.

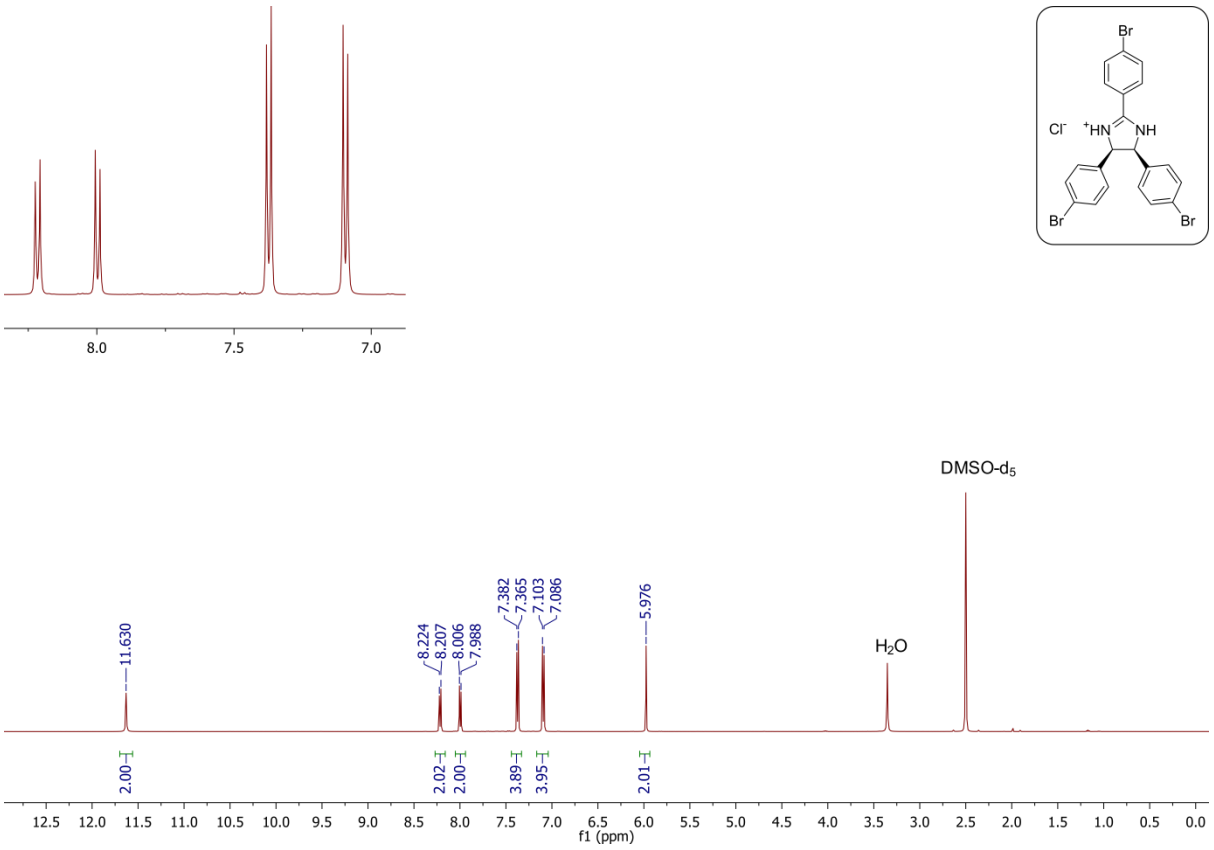


Fig. S17 ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **8** with the structure in insert.

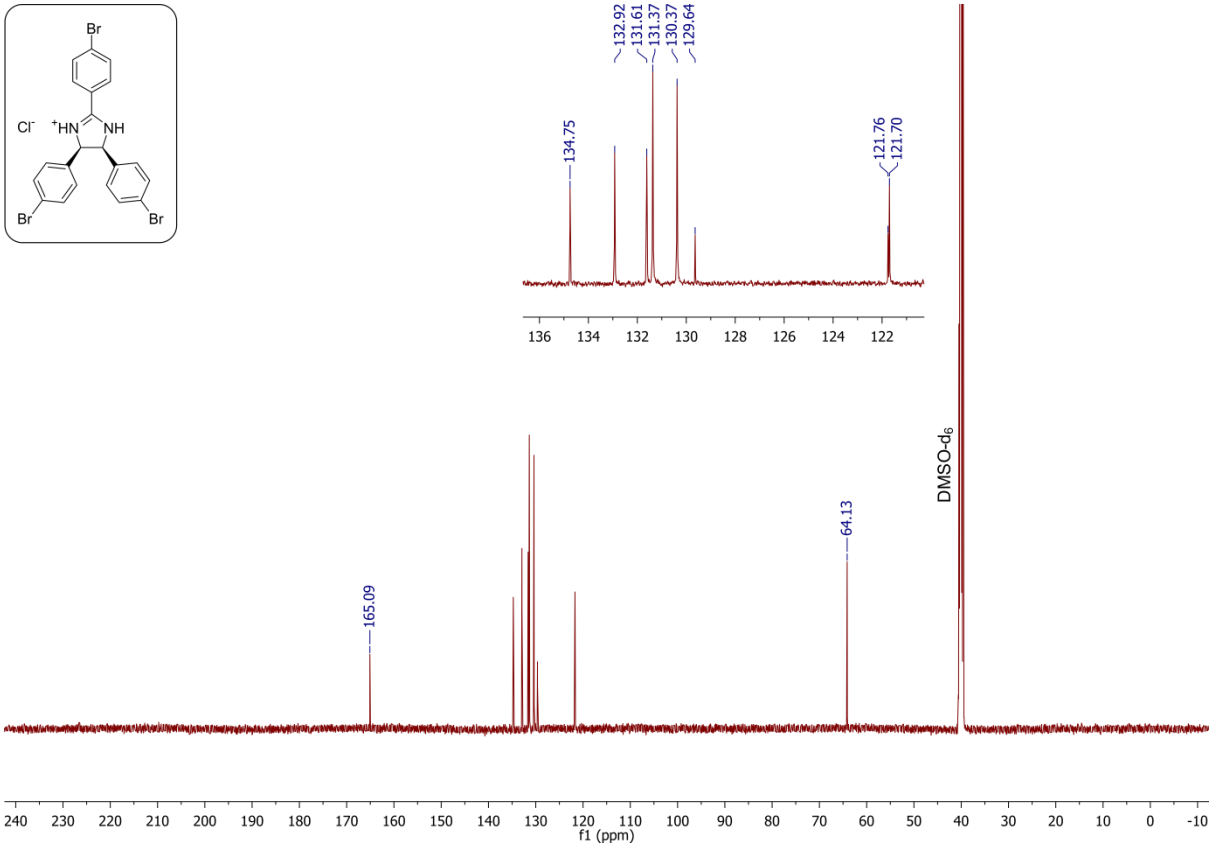


Fig. S18 ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **8** with the structure in insert.

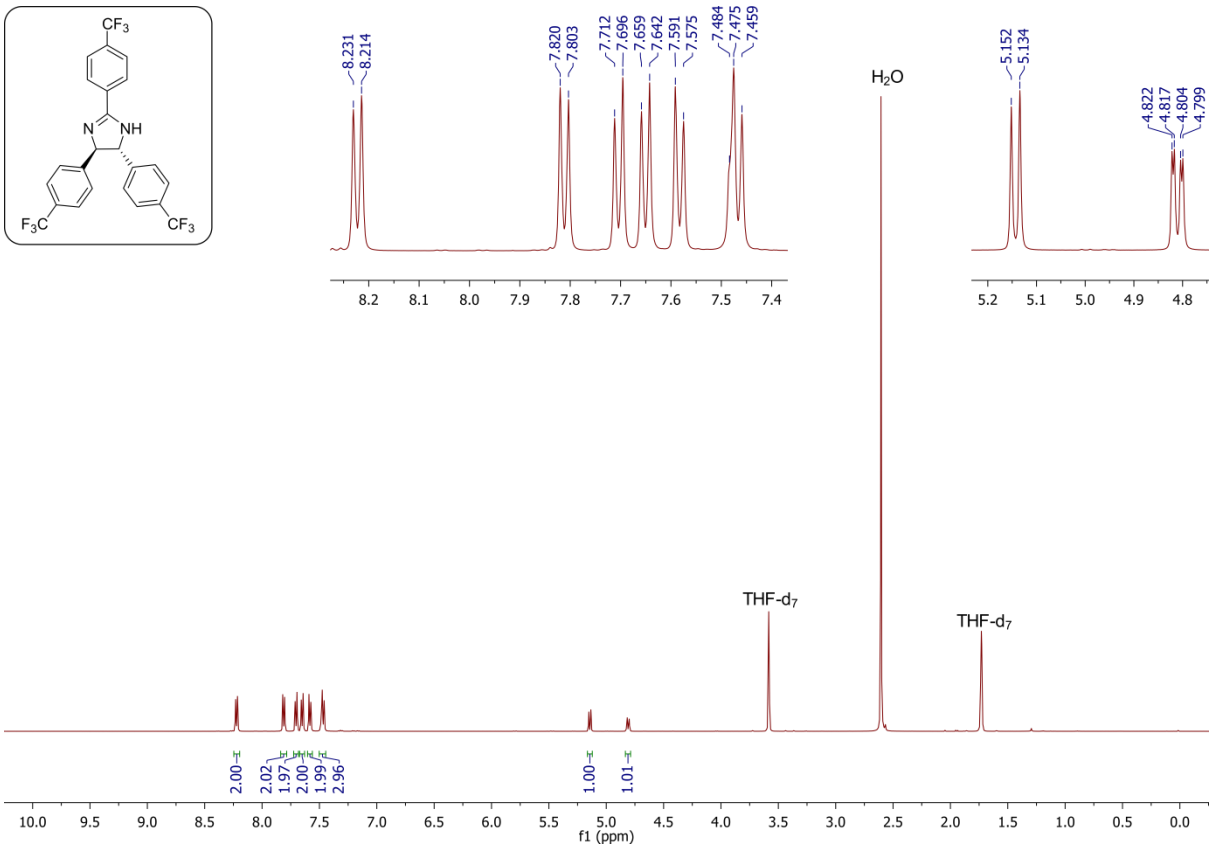


Fig. S19 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **9** with the structure in insert.

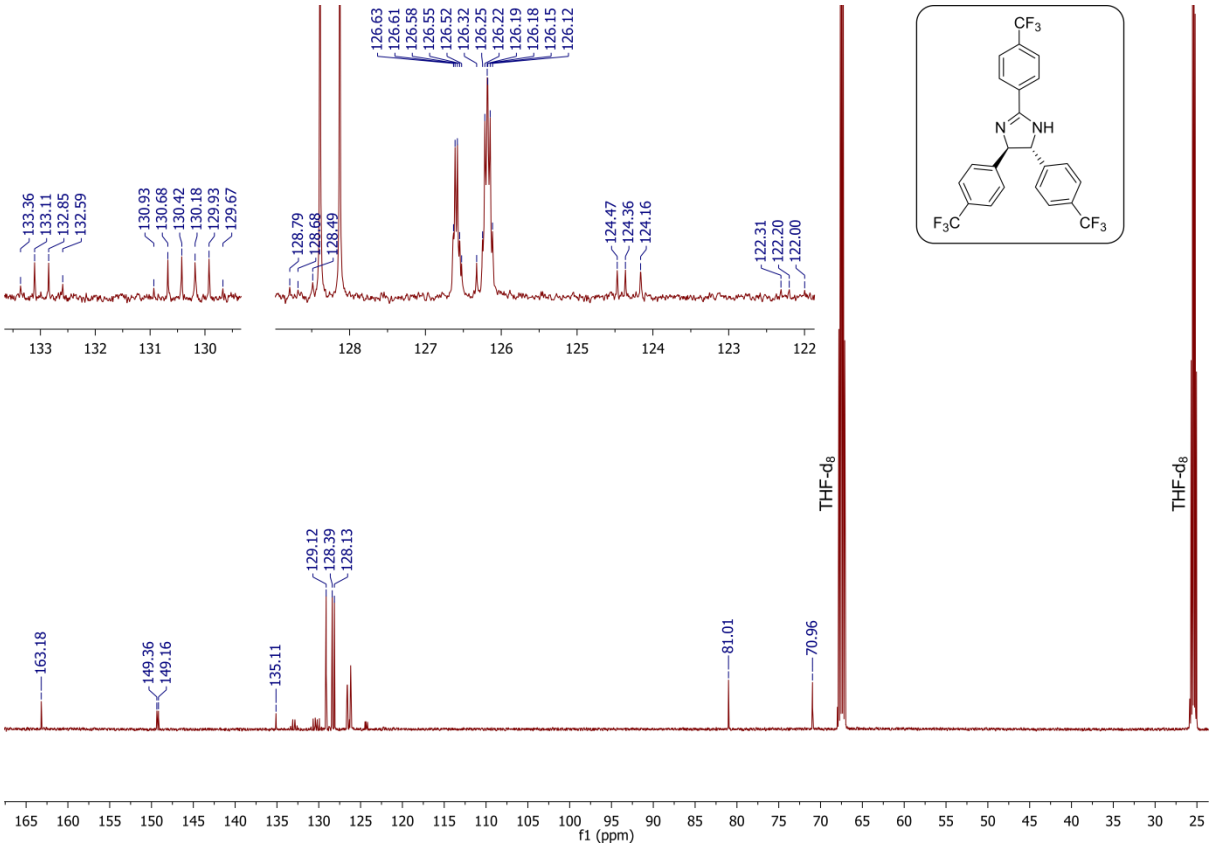


Fig. S20 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **9** with the structure in insert.

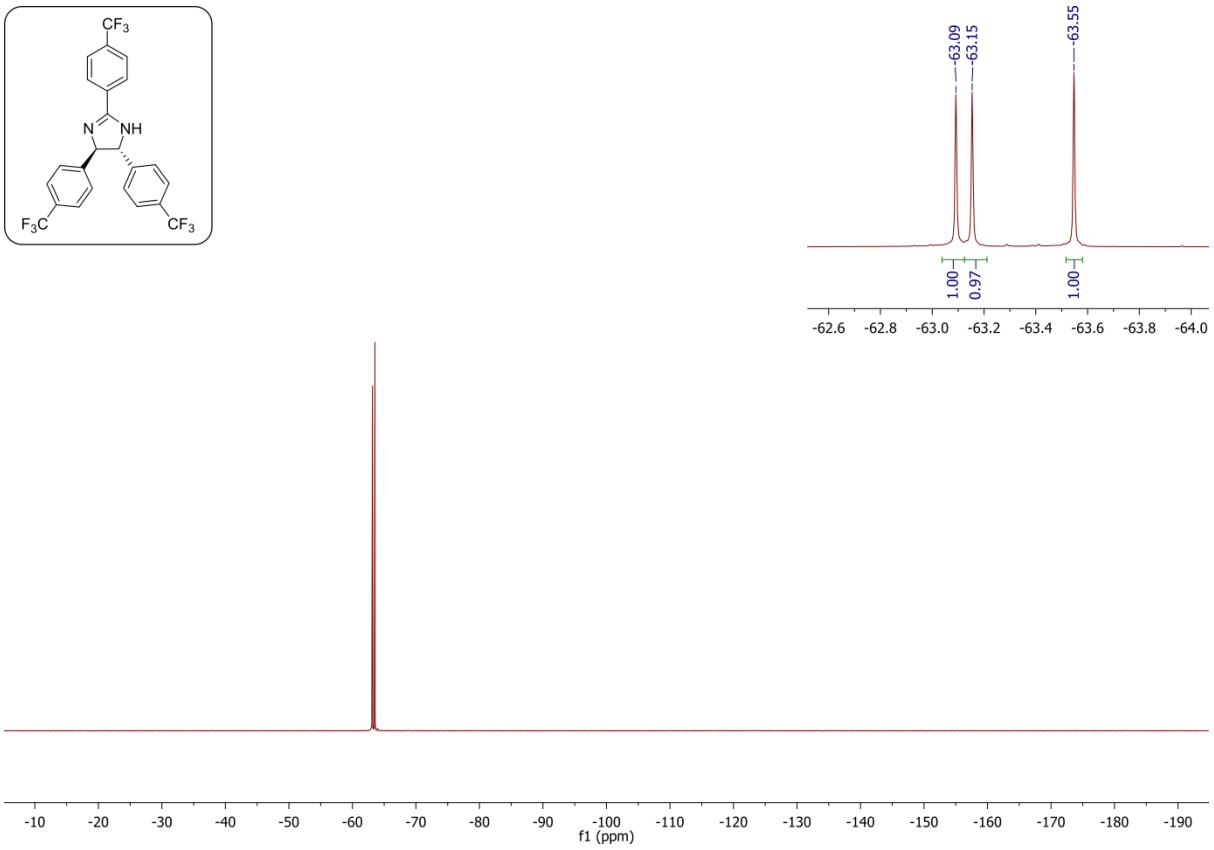


Fig. S21 ^{19}F NMR (471 MHz, THF-d_8) spectrum of **9** with the structure in insert.

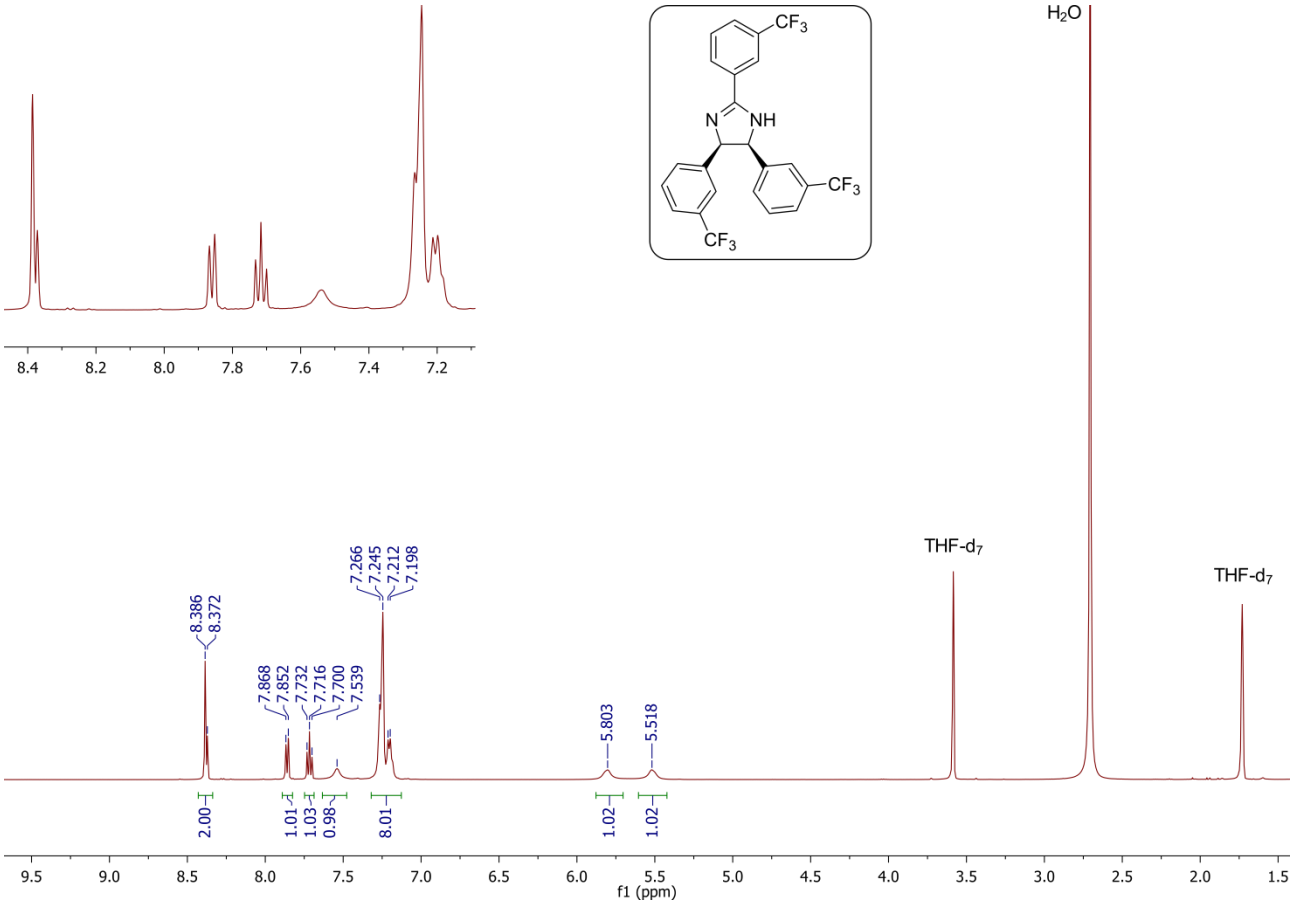


Fig. S22 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **10** with the structure in insert.

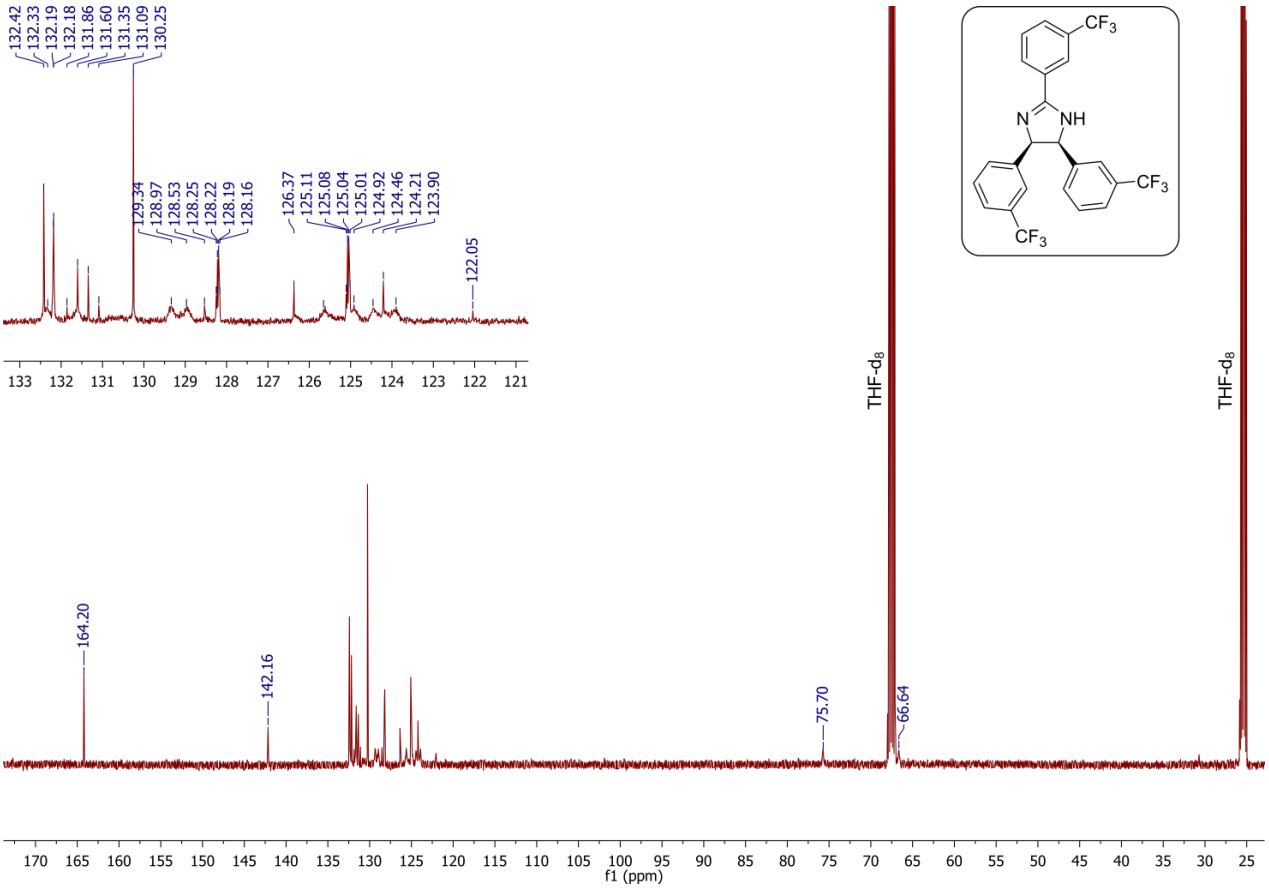


Fig. S23 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **10** with the structure in insert.

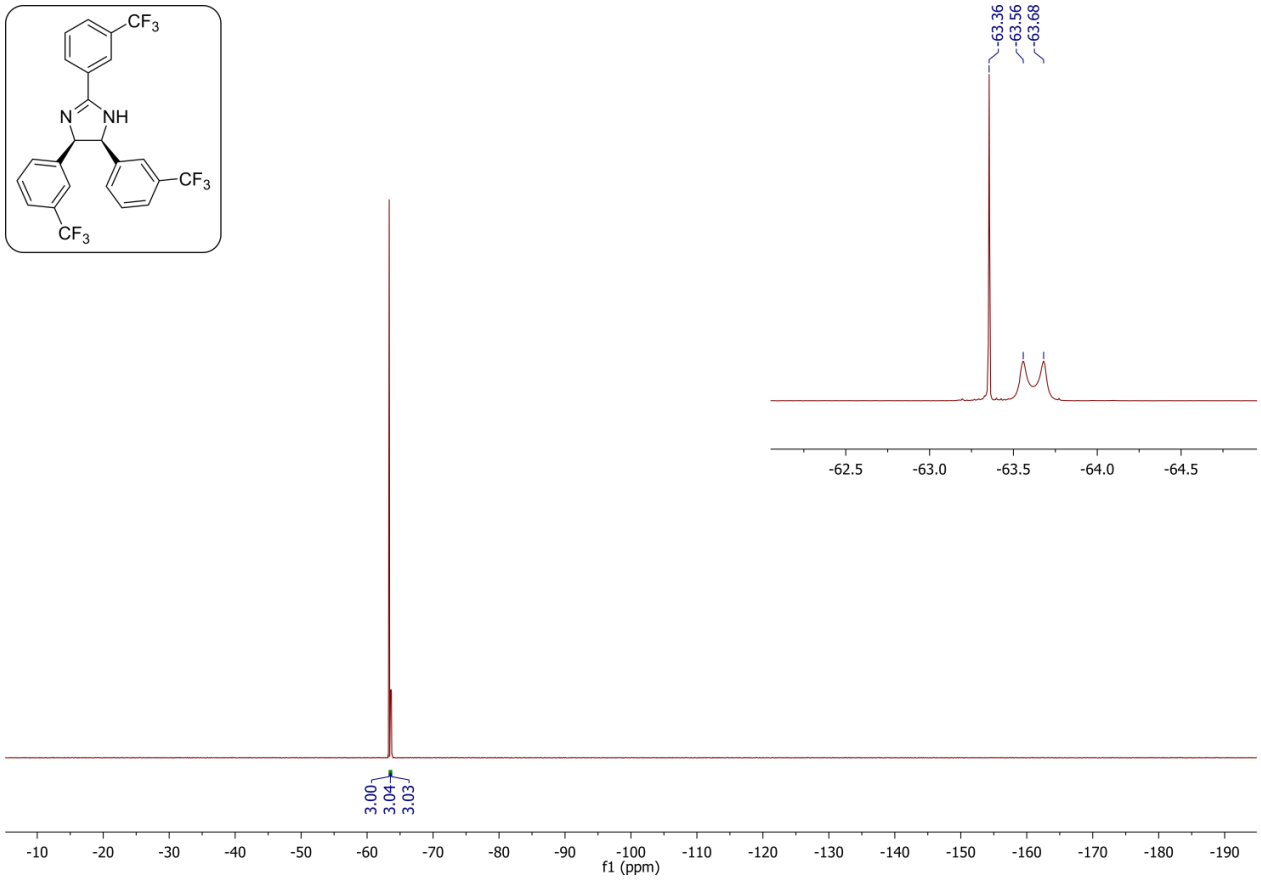


Fig. S24 ^{19}F NMR (471 MHz, THF-d_8) spectrum of **10** with the structure in insert.

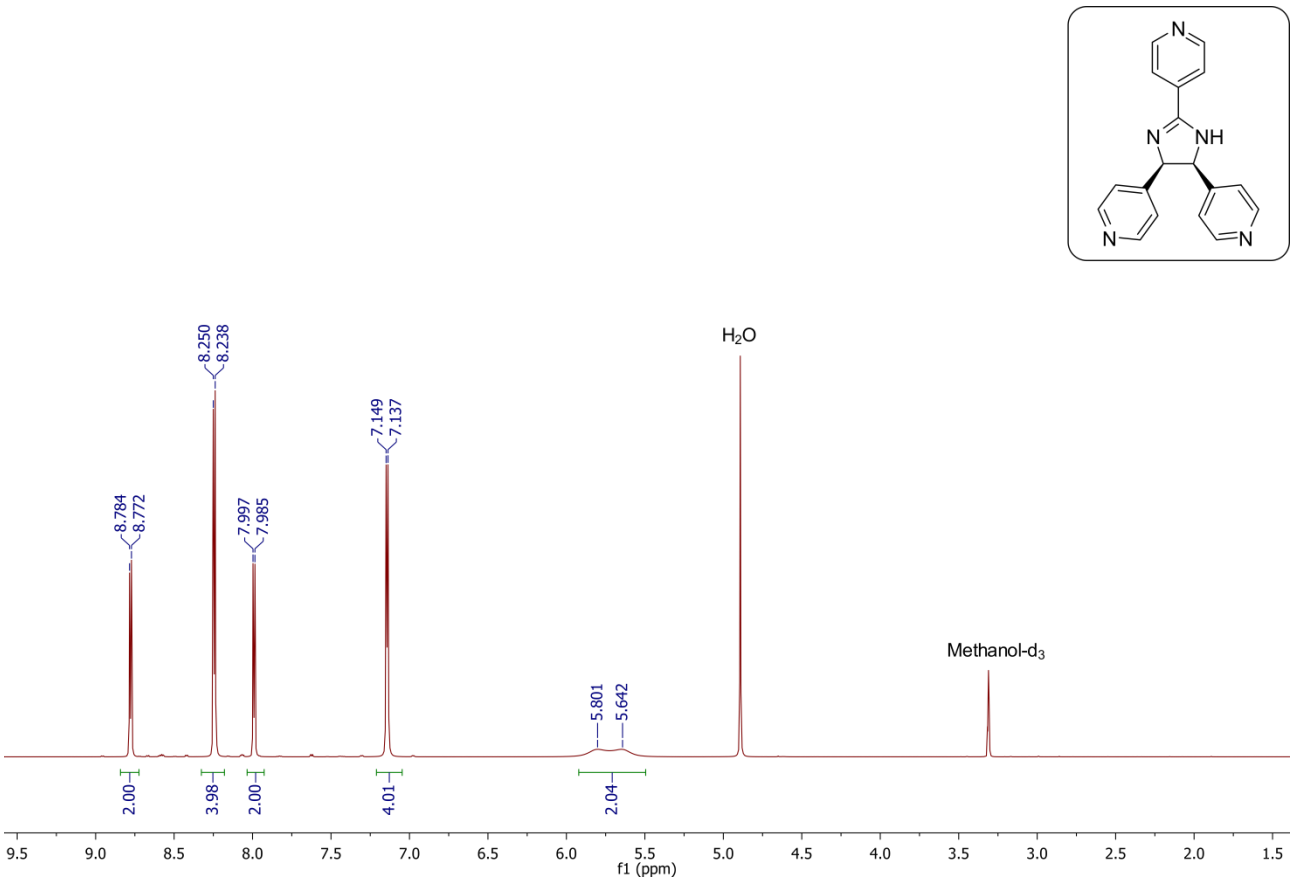


Fig. S25 ^{1}H NMR (500 MHz, CD_3OD) spectrum of **11** with the structure in insert.

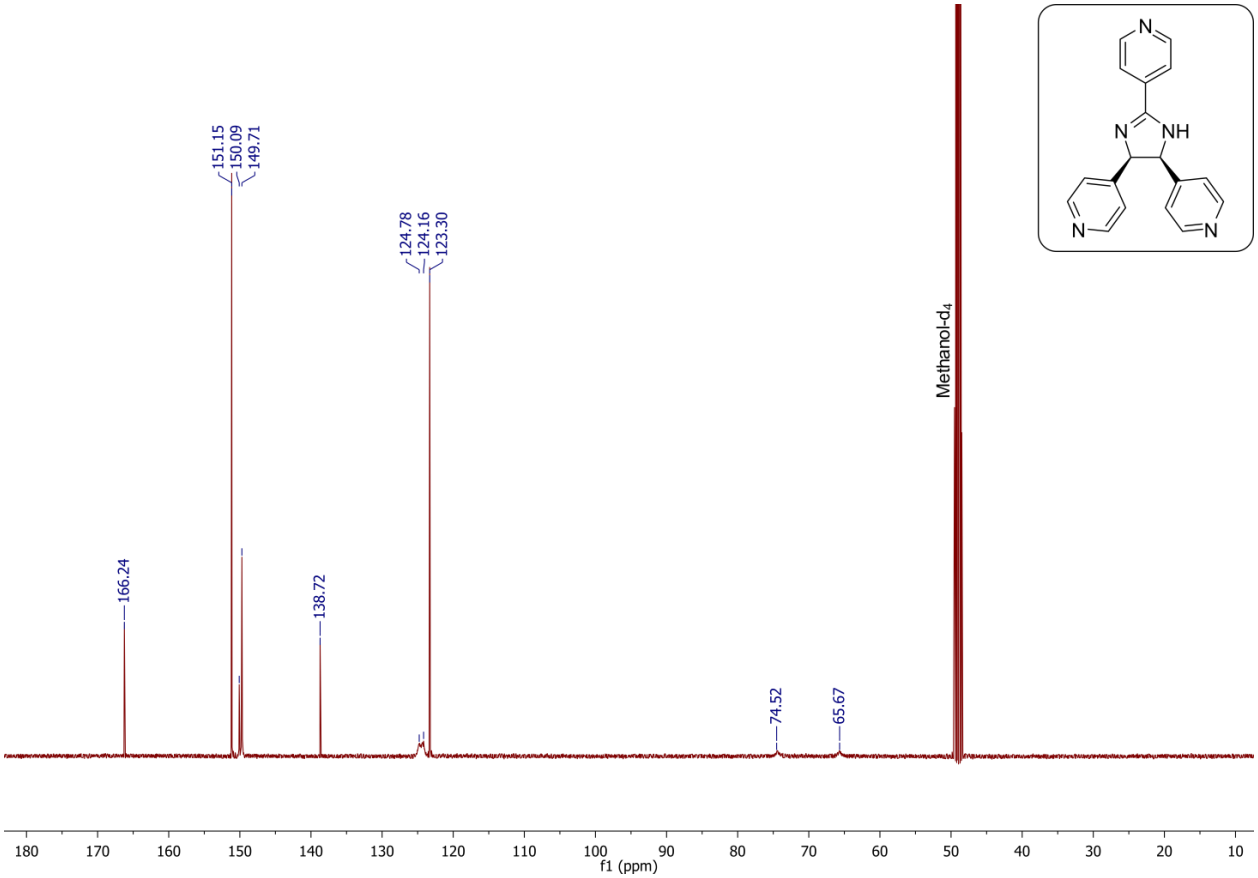


Fig. S26 ^{13}C NMR (126 MHz, CD_3OD) spectrum of **11** with the structure in insert.

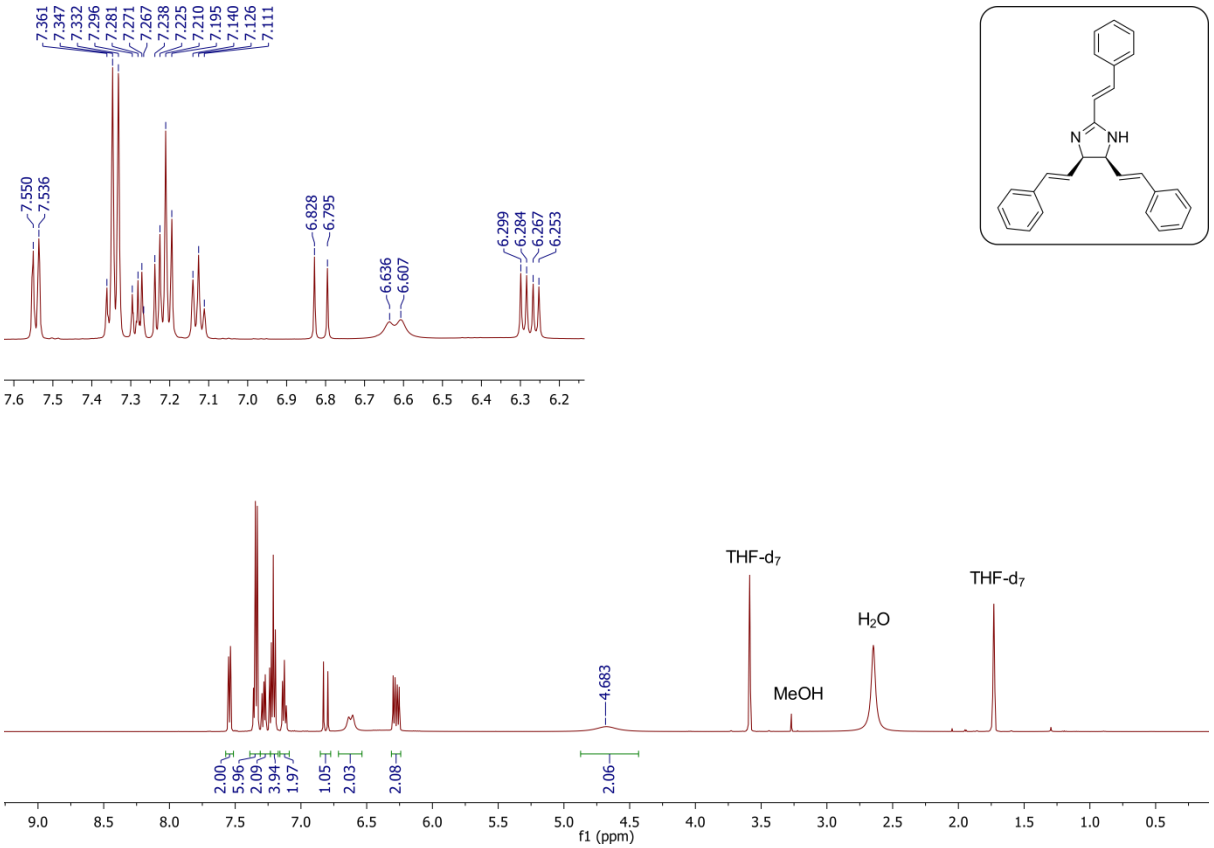


Fig. S27 ^{1}H NMR (500 MHz, THF-d_8) spectrum of **12** with the structure in insert.

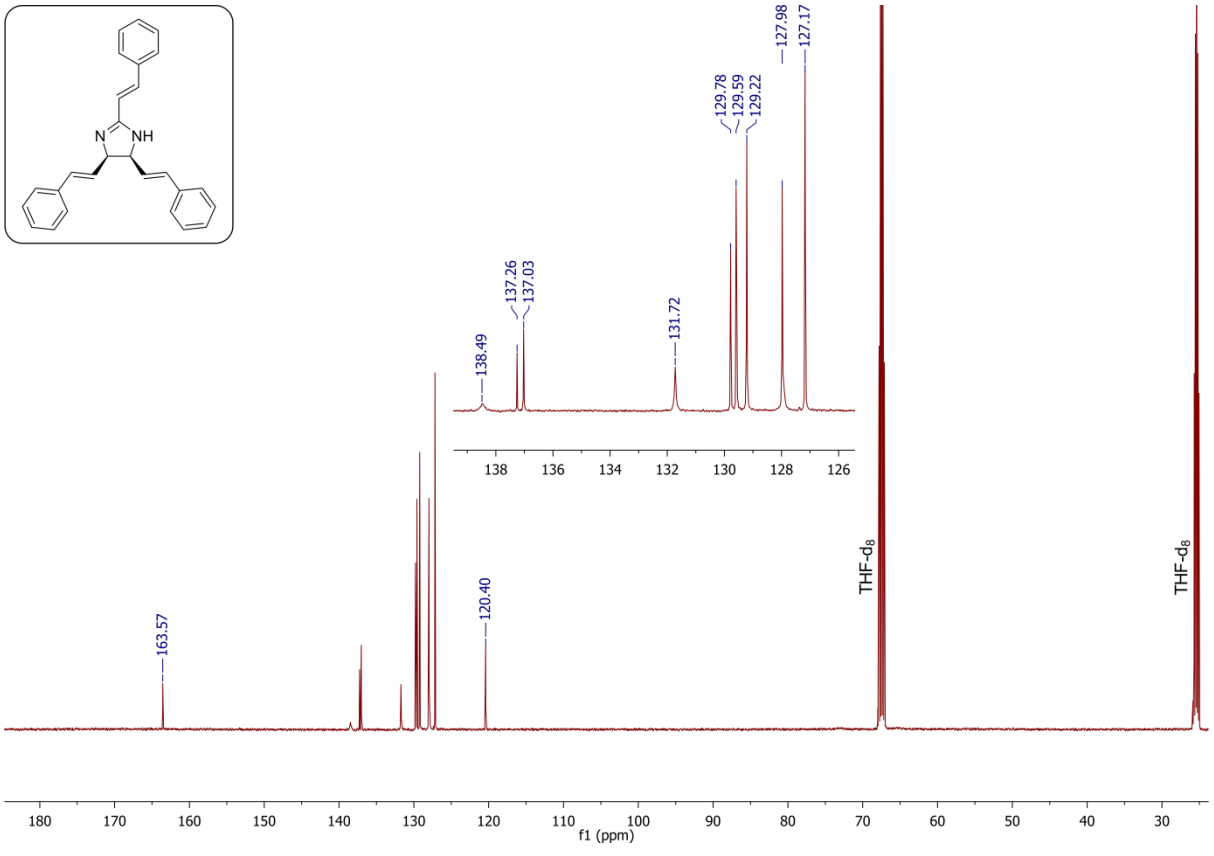


Fig. S28 ^{13}C NMR (126 MHz, THF-d_8) spectrum of **12** with the structure in insert.

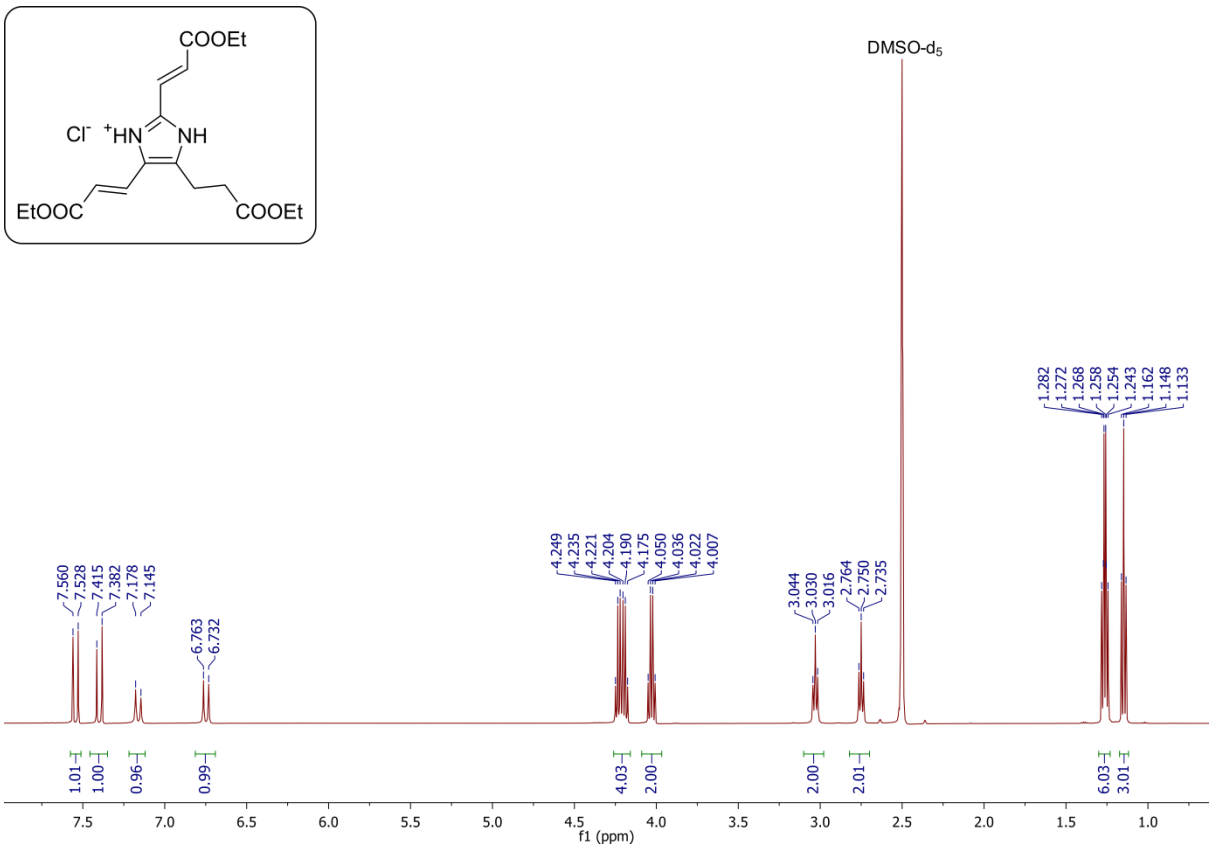


Fig. S29 ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **13** with the structure in insert.

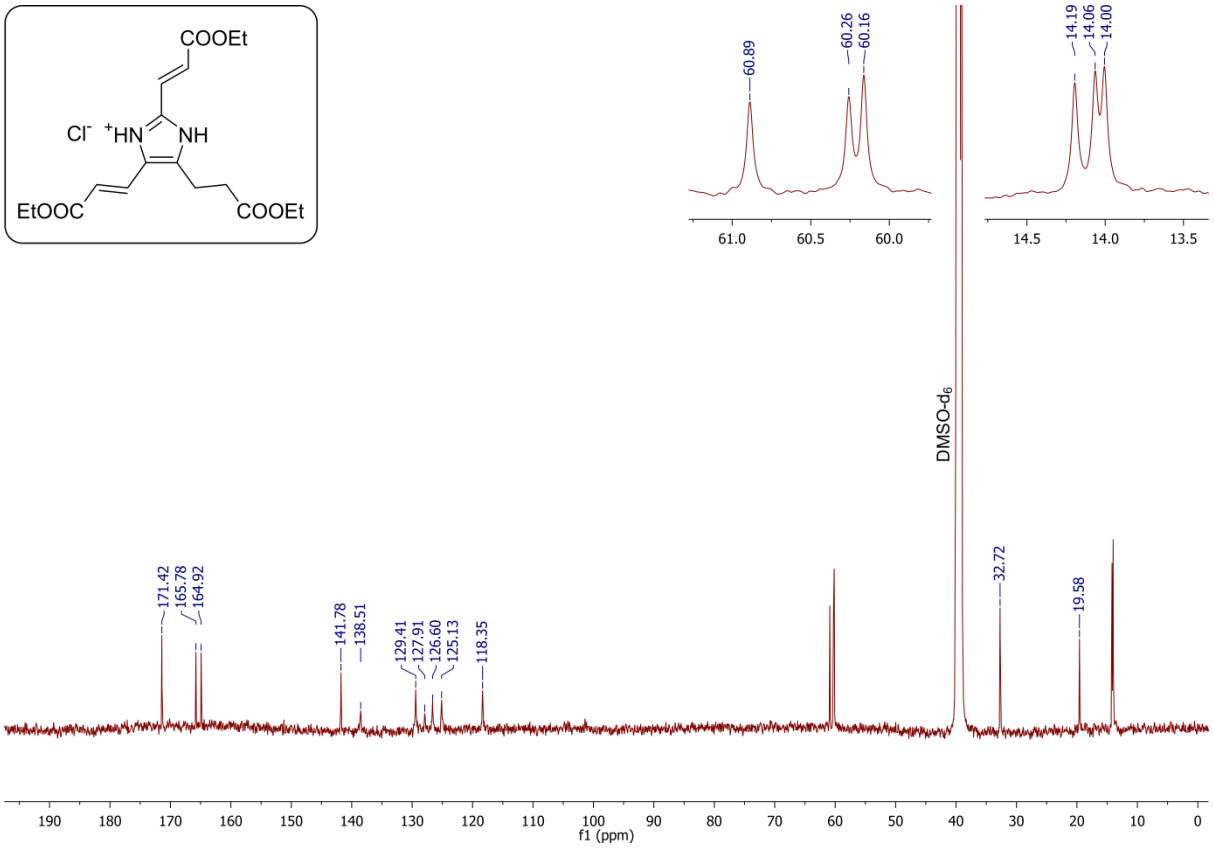


Fig. S30 ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **13** with the structure in insert.

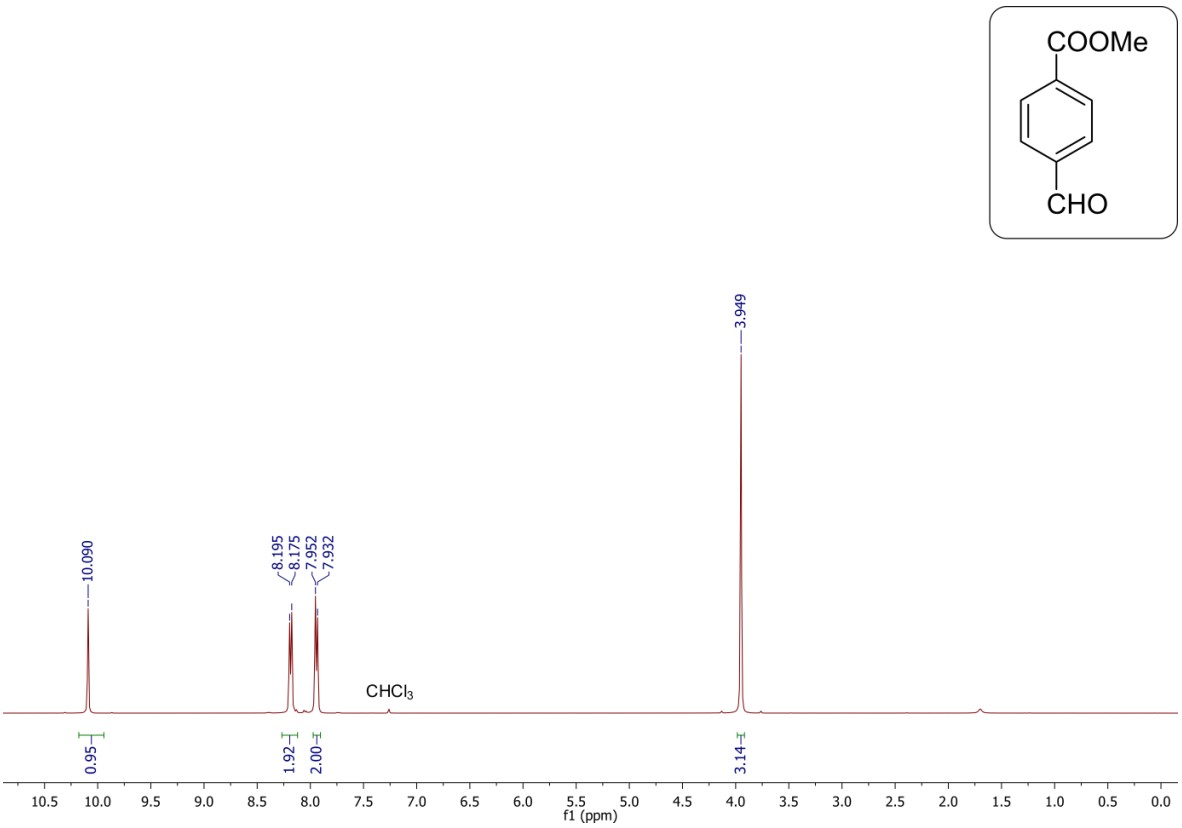


Fig. S31 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of methyl 4-formylbenzoate with the structure in insert.

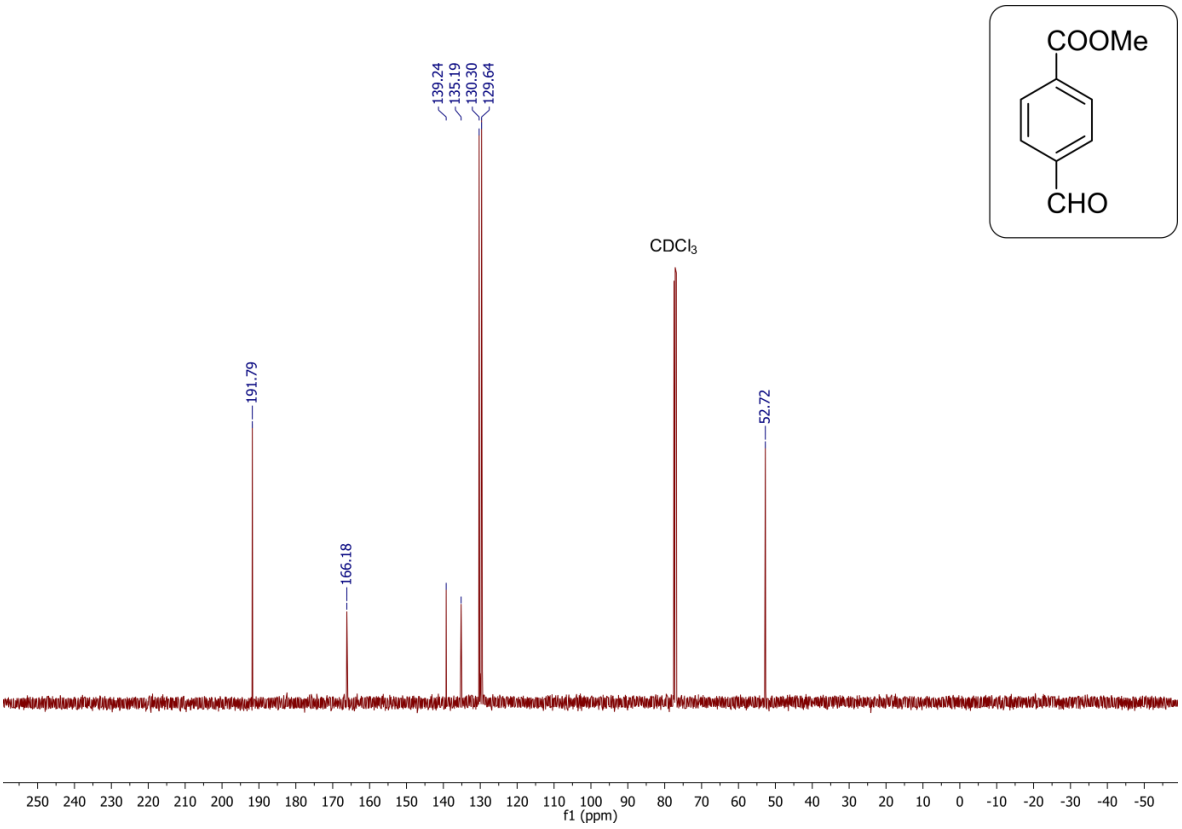


Fig. S32 ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of methyl 4-formylbenzoate with the structure in insert.

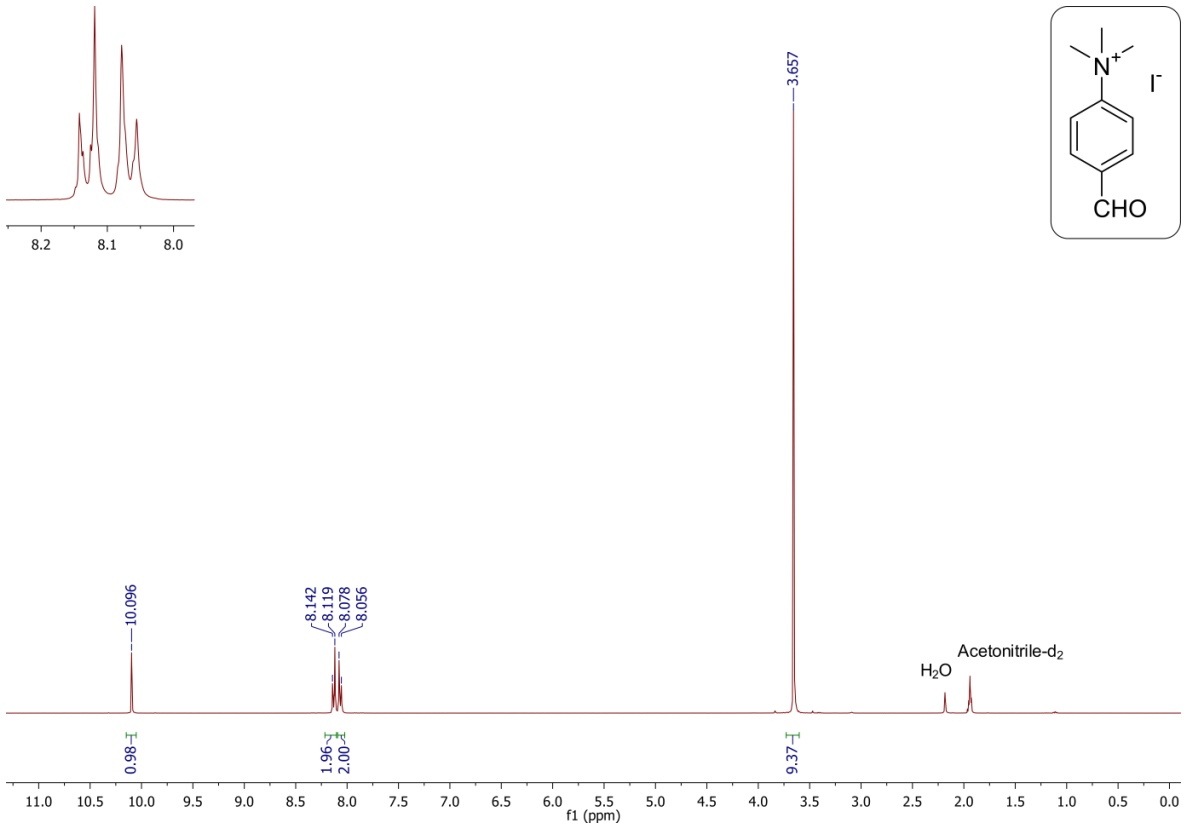


Fig. S33 ^{1}H NMR (500 MHz, CD_3CN) spectrum of 4-formyl-*N*,*N*,*N*-trimethylanilinium iodide with the structure in insert.

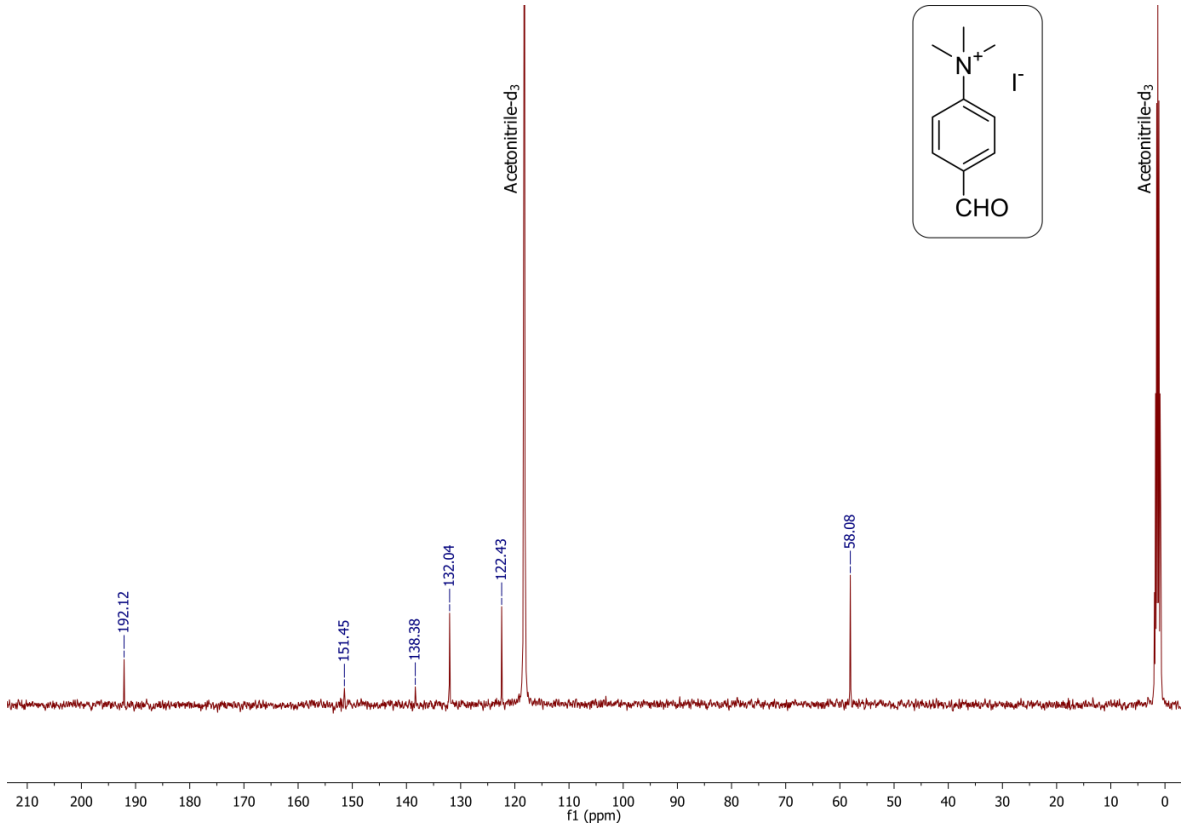


Fig. S34 ^{13}C NMR (126 MHz, CD_3CN) spectrum of 4-formyl-*N*,*N*,*N*-trimethylanilinium iodide with the structure in insert.

3. Mass spectra

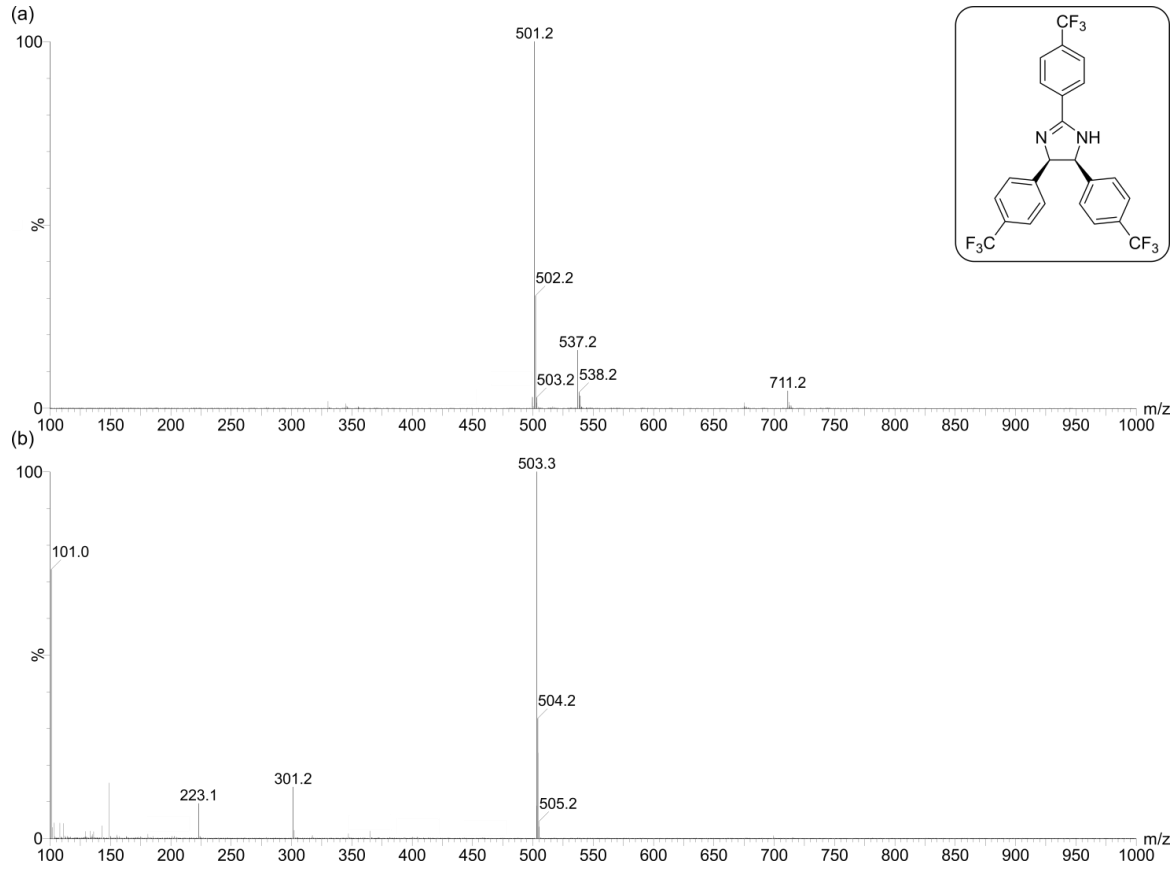


Fig. S35 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **1** with the structure in insert.

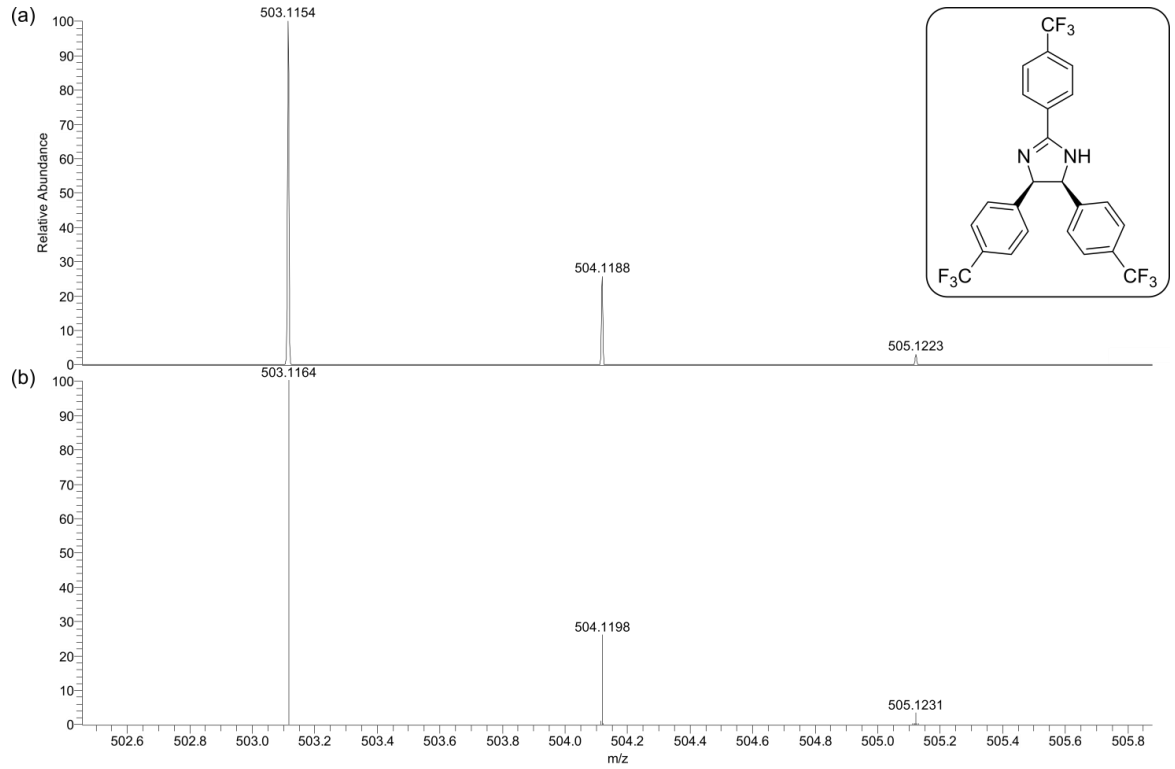


Fig. S36 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **1** in insert.

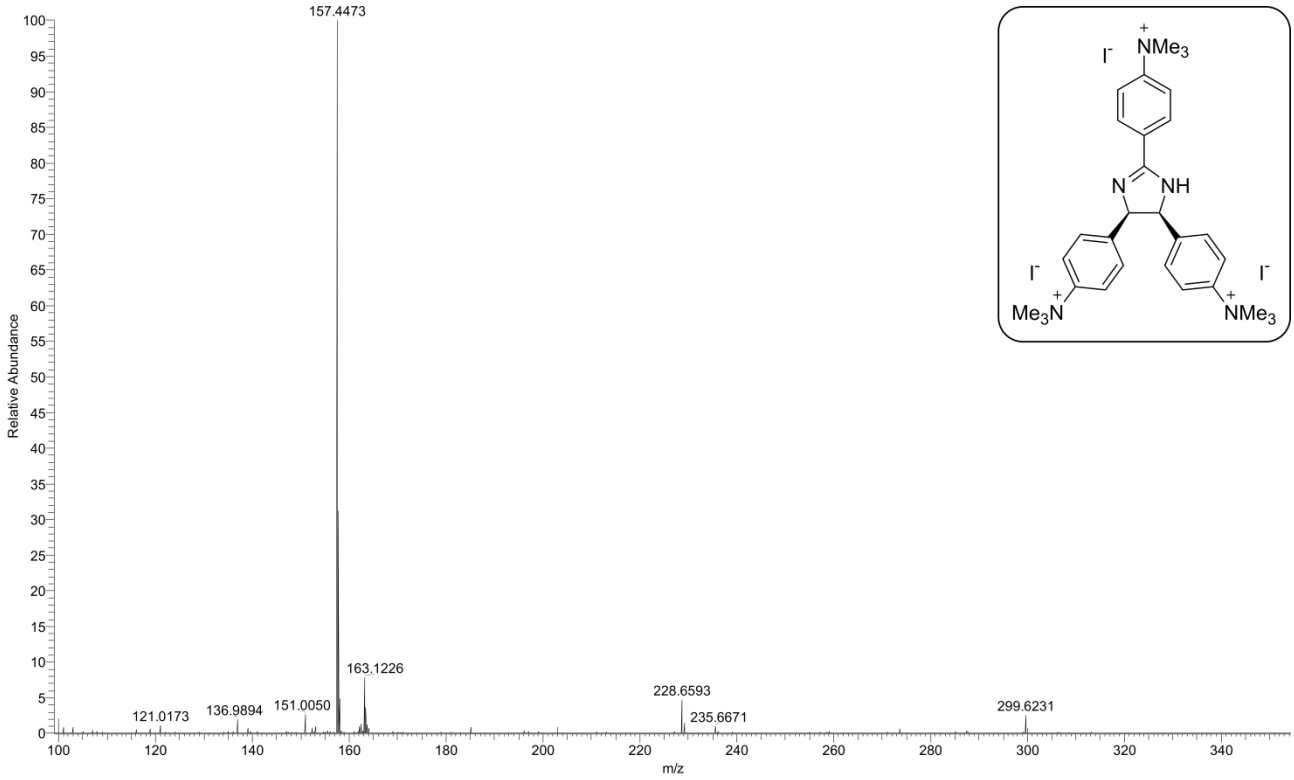


Fig. S37 ESI+/Orbitrap mass spectrum of **2** with the structure in insert.

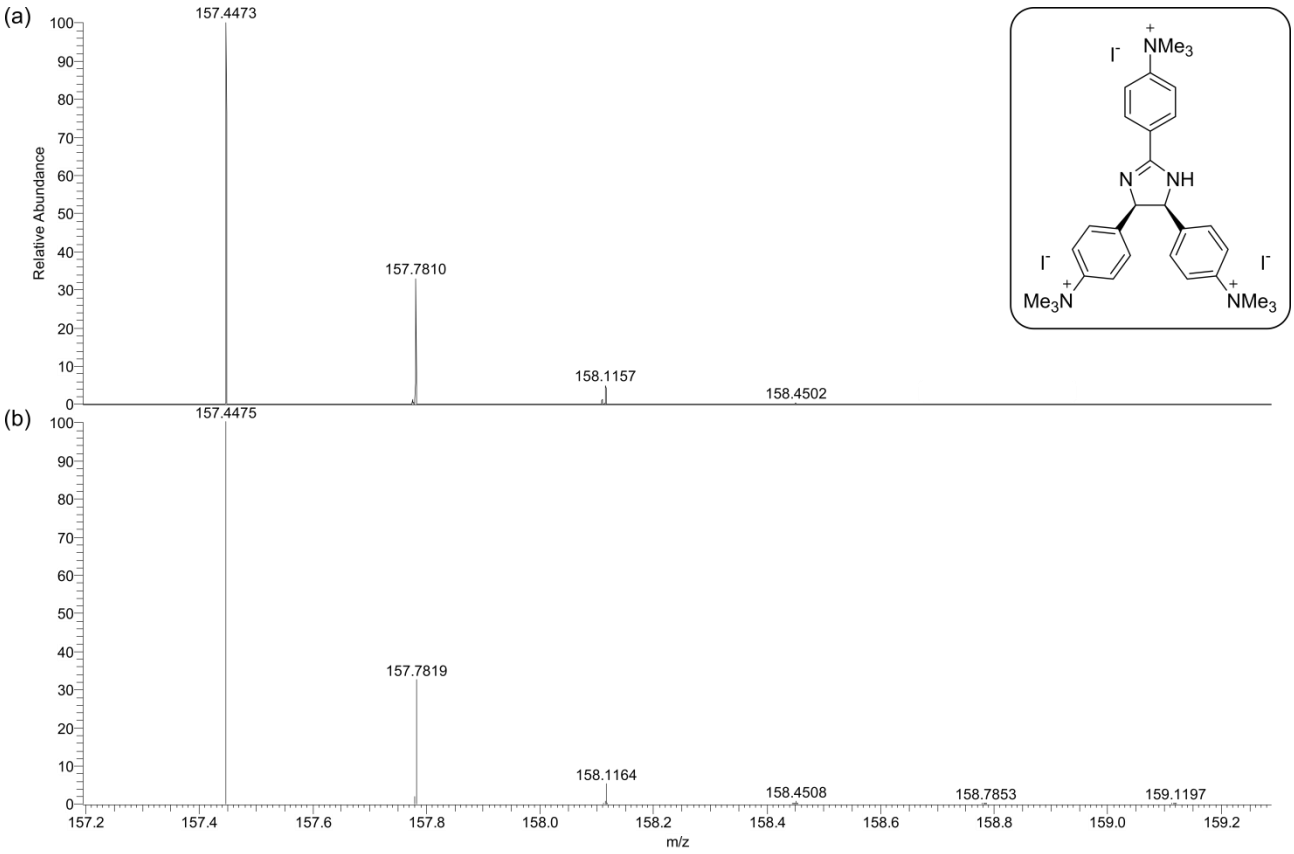


Fig. S38 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M]^{3+}$ ion with the structure of **2** in insert.

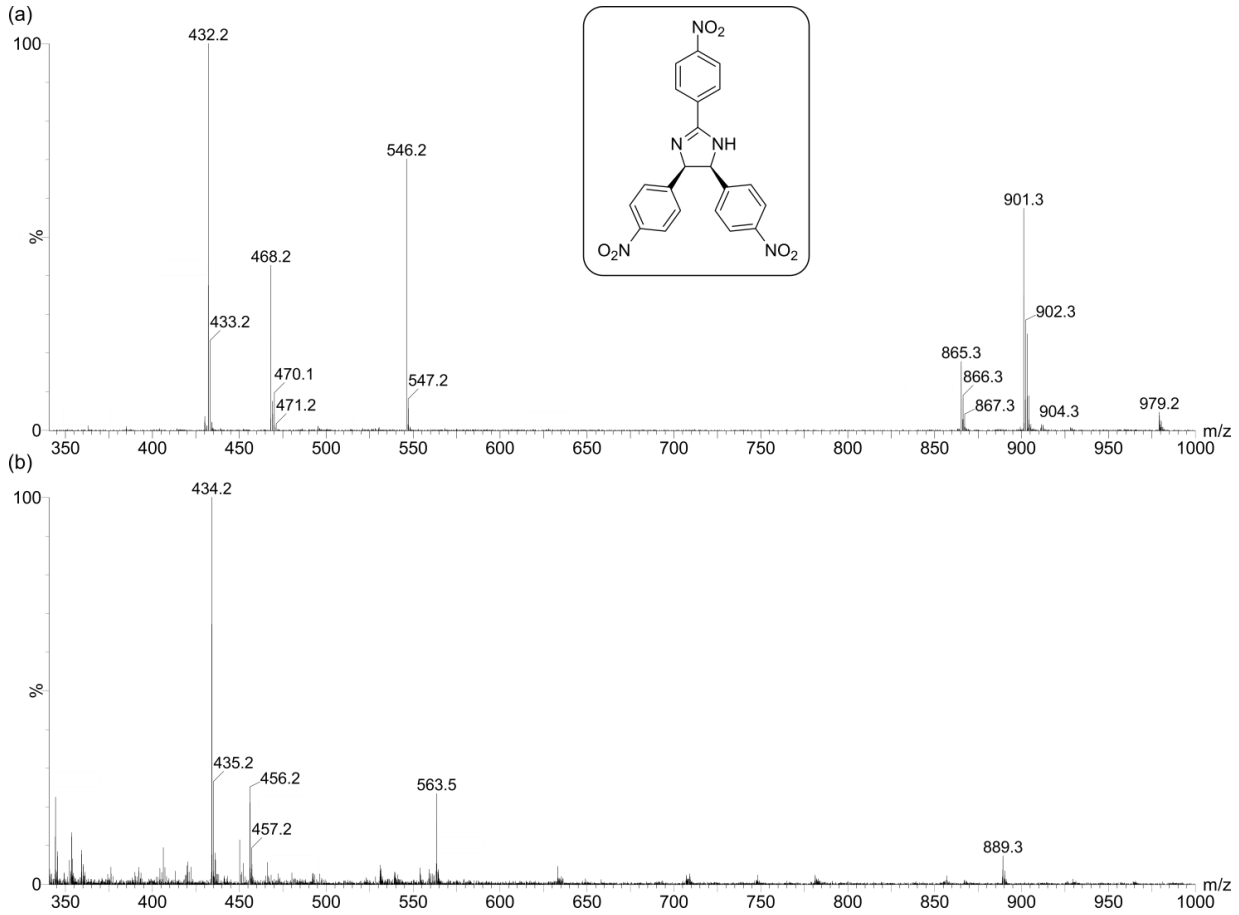


Fig. S39 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **3** with the structure in insert.

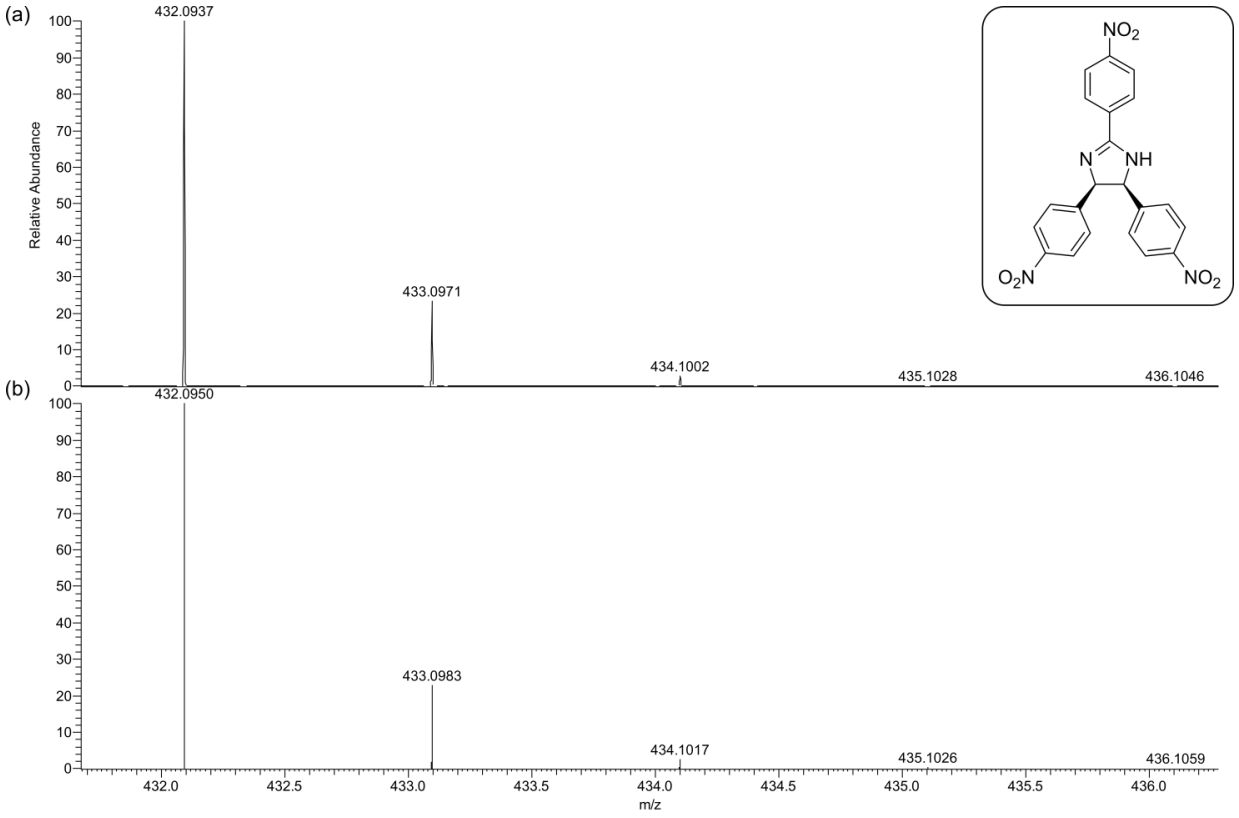


Fig. S40 (a) Observed ESI– high resolution mass spectrum and (b) calculated isotopic distribution of the $[M–H]^-$ ion with the structure of **3** in insert.

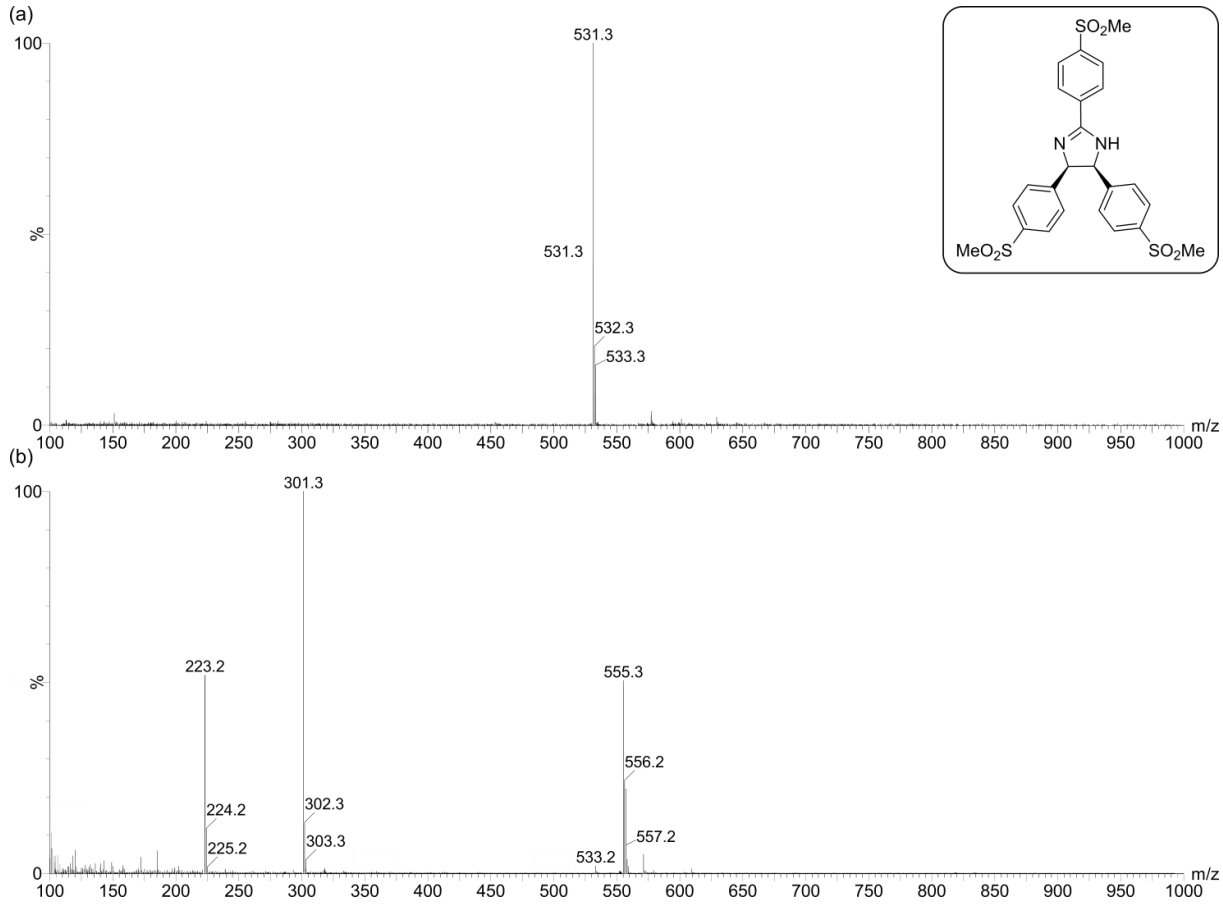


Fig. S41 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **4** with the structure in insert.

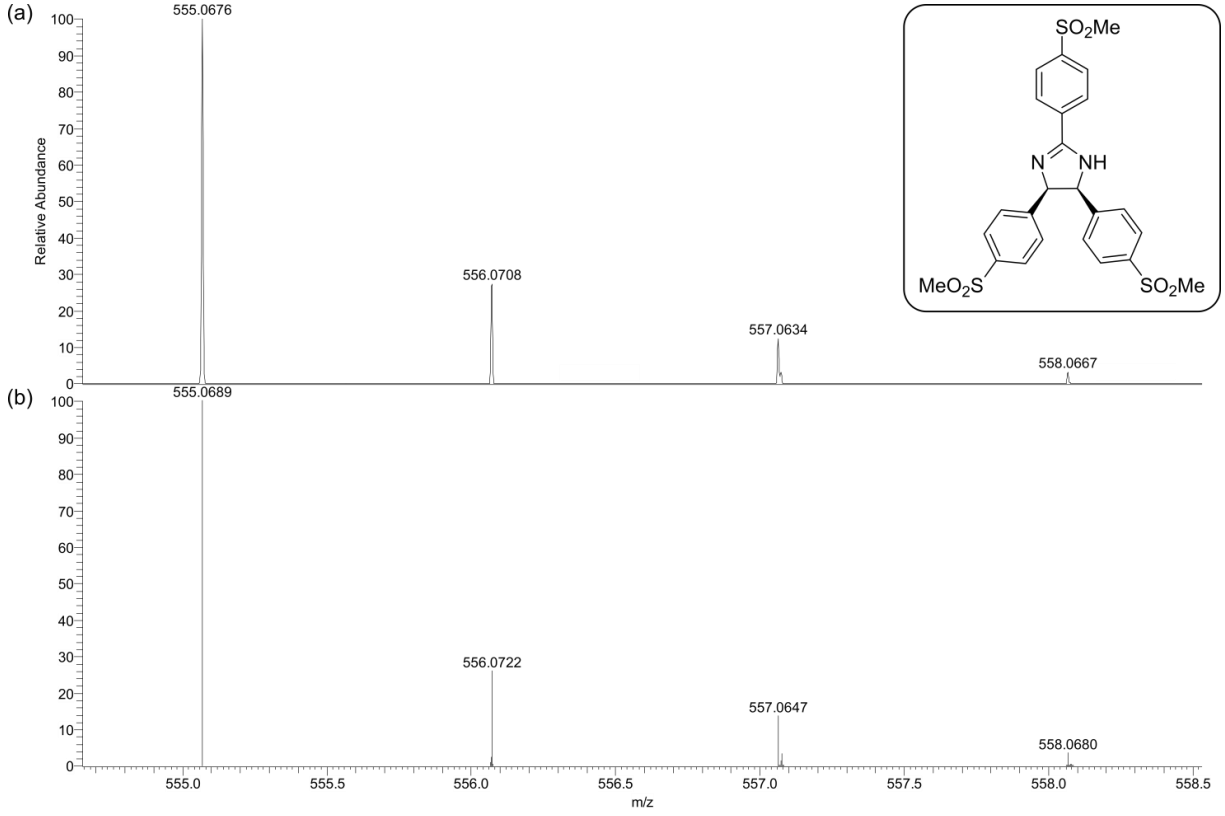


Fig. S42 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+Na]^+$ adduct with the structure of **4** in insert.

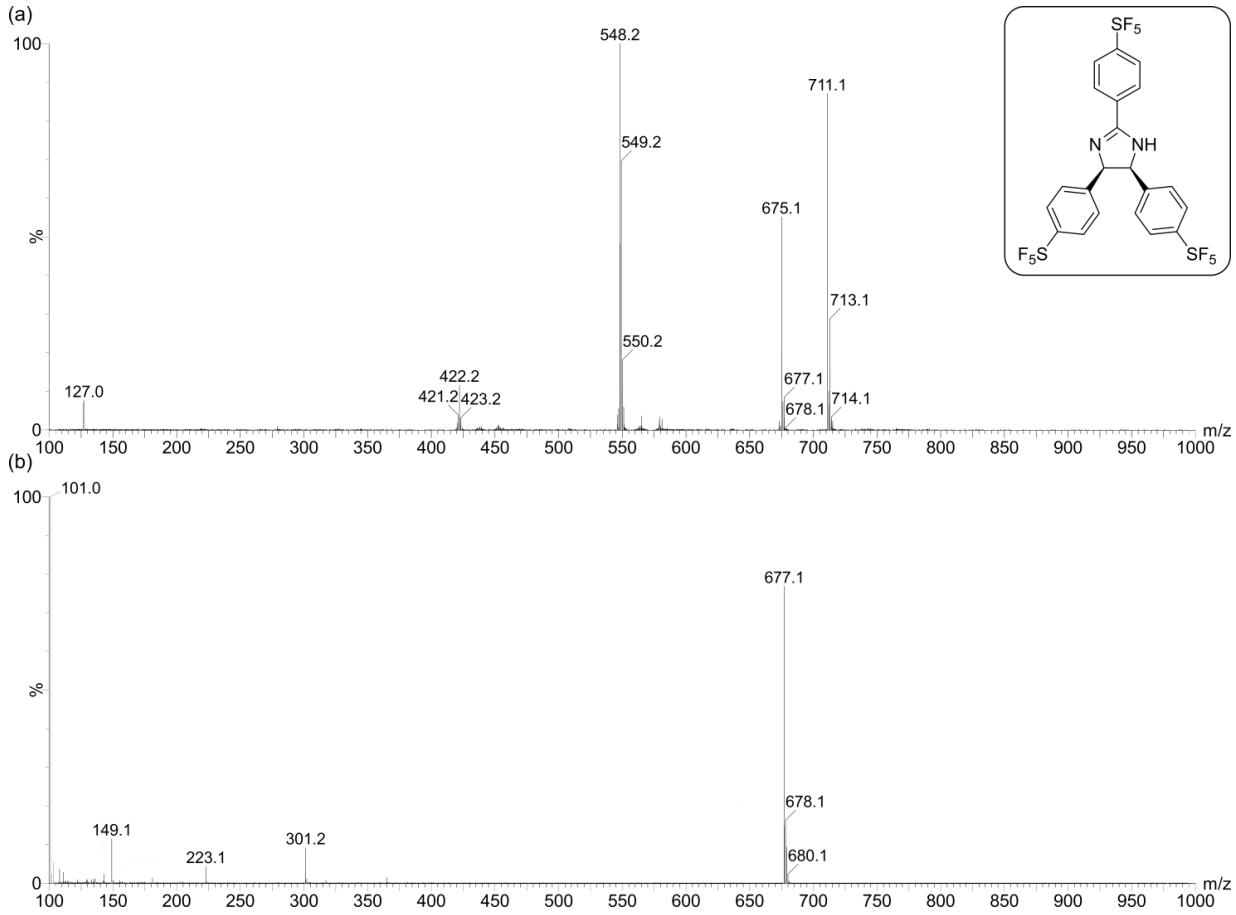


Fig. S43 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **5** with the structure in insert.

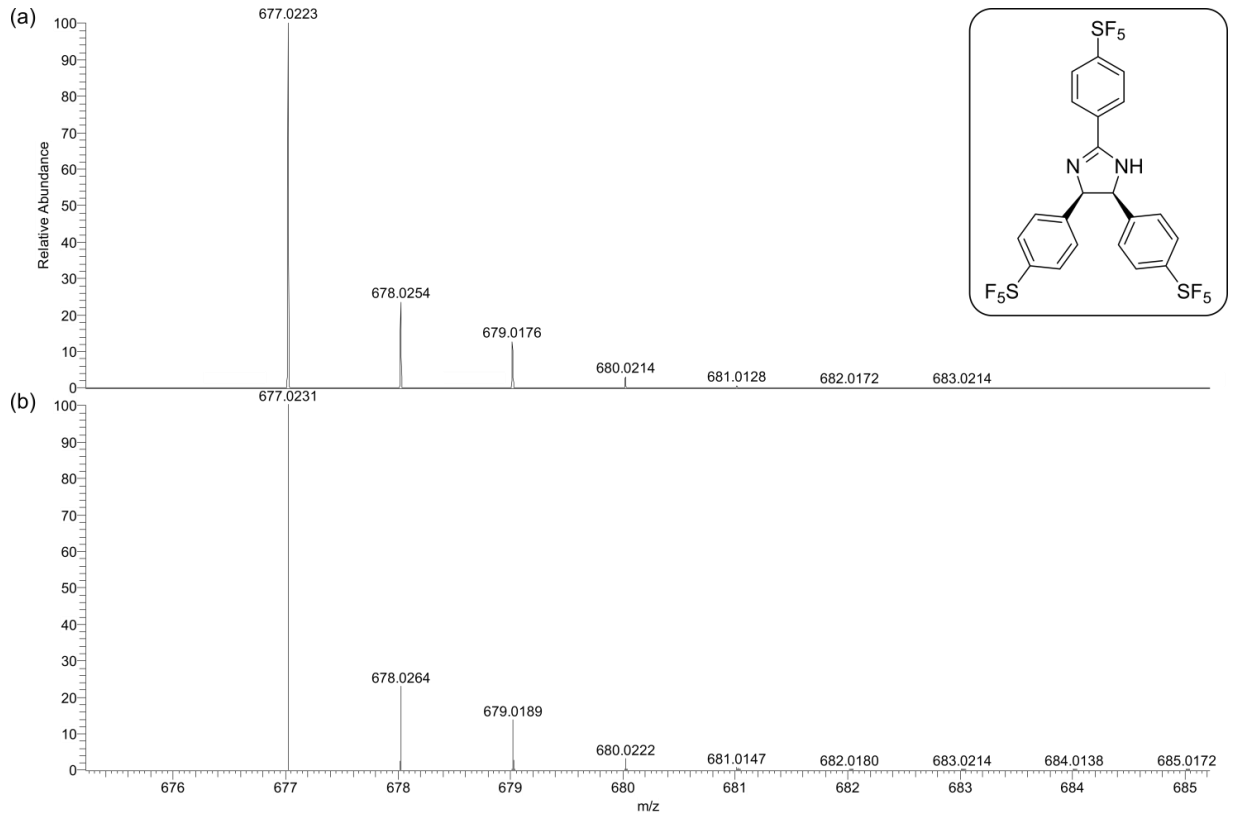


Fig. S44 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **5** in insert.

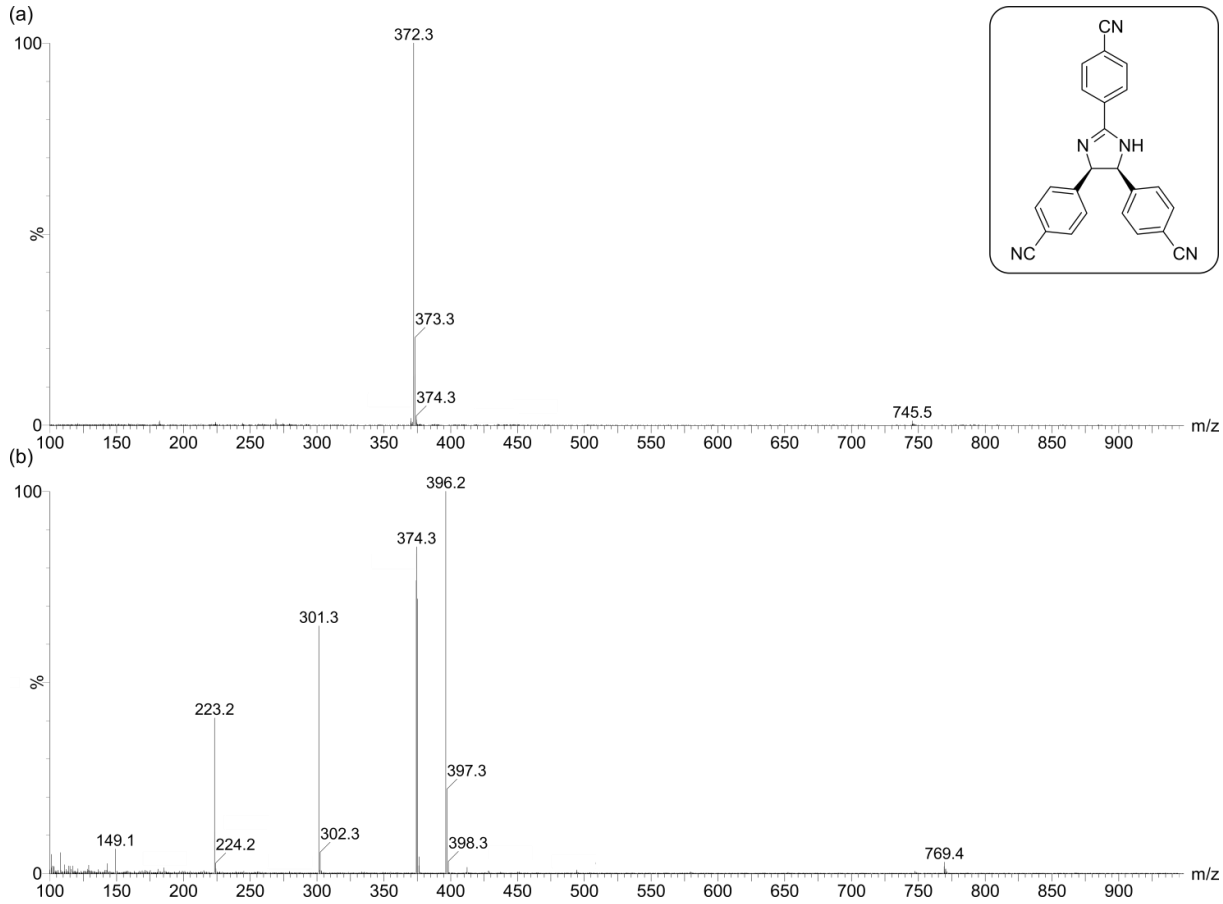


Fig. S45 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **6** with the structure in insert.

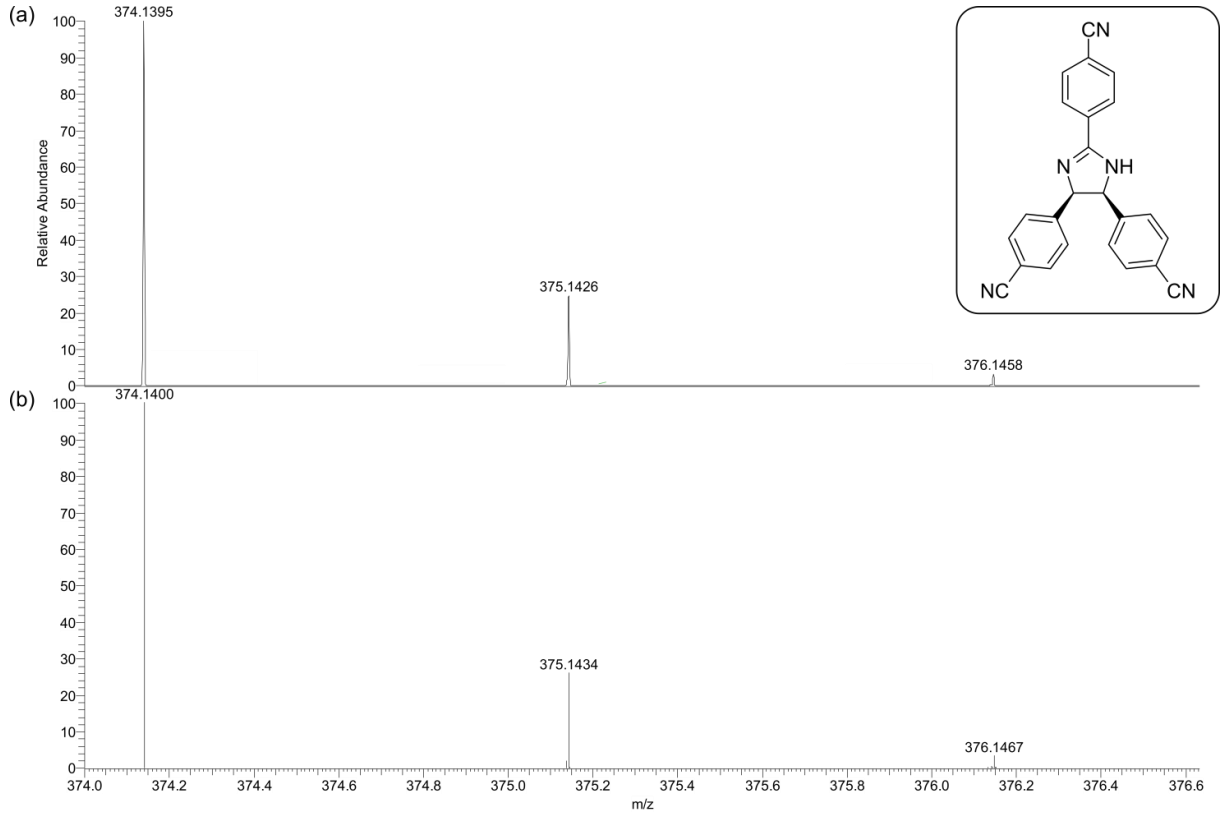


Fig. S46 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **6** in insert.

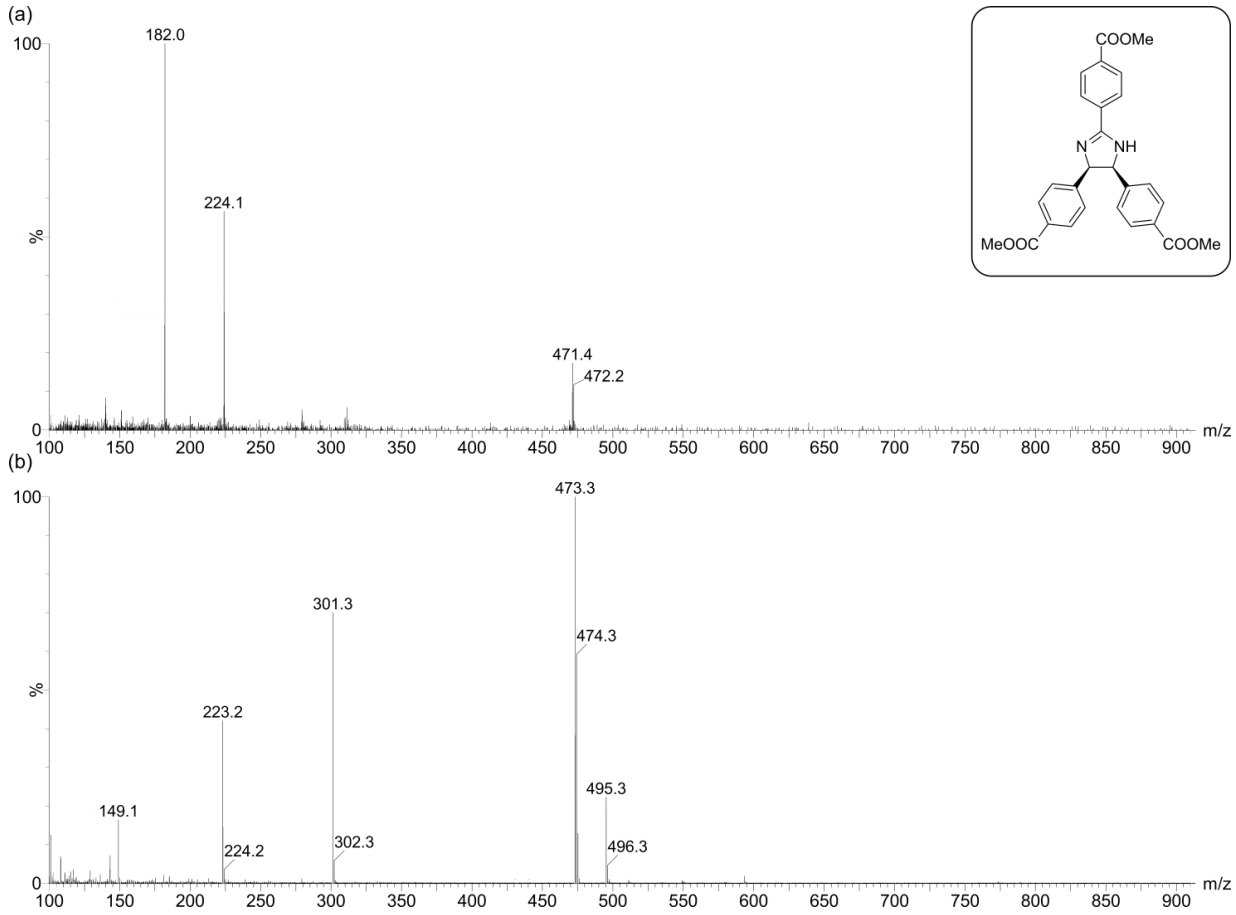


Fig. S47 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **7** with the structure in insert.

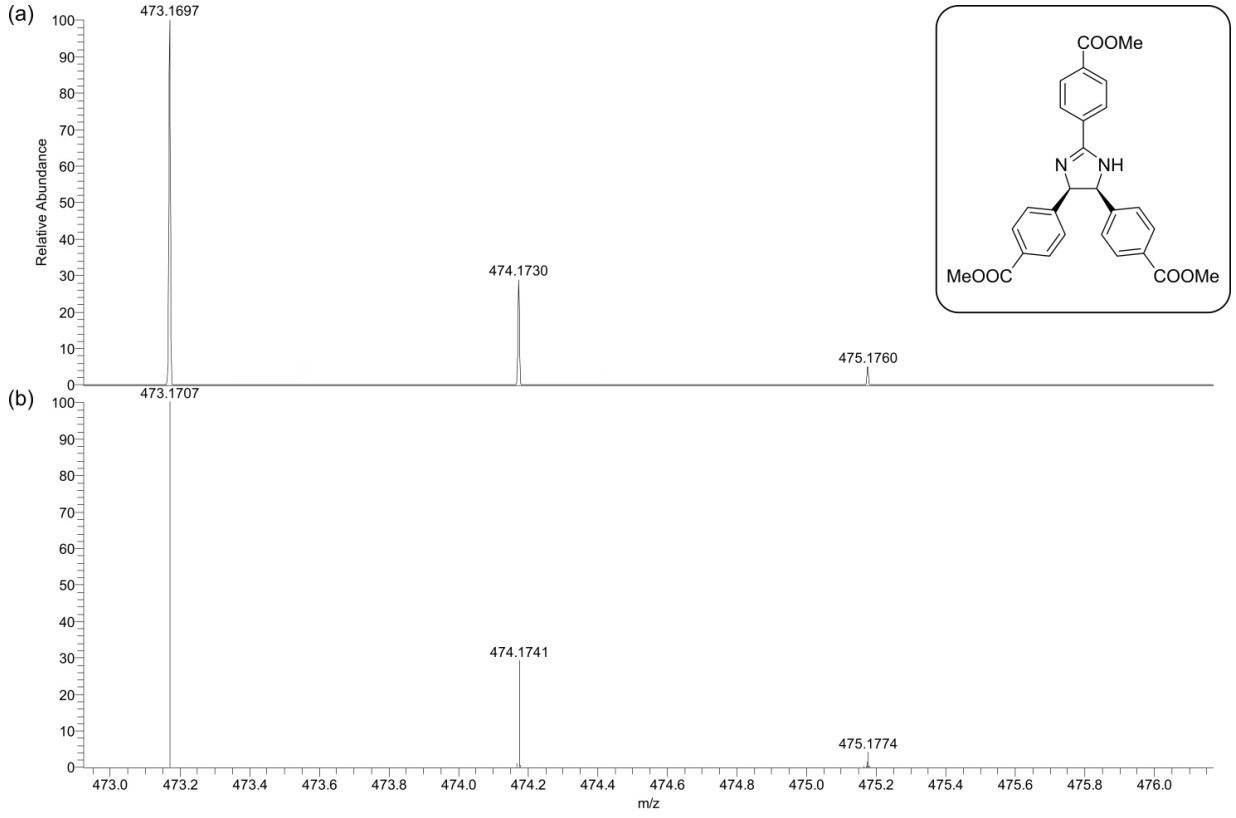


Fig. S48 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **7** in insert.

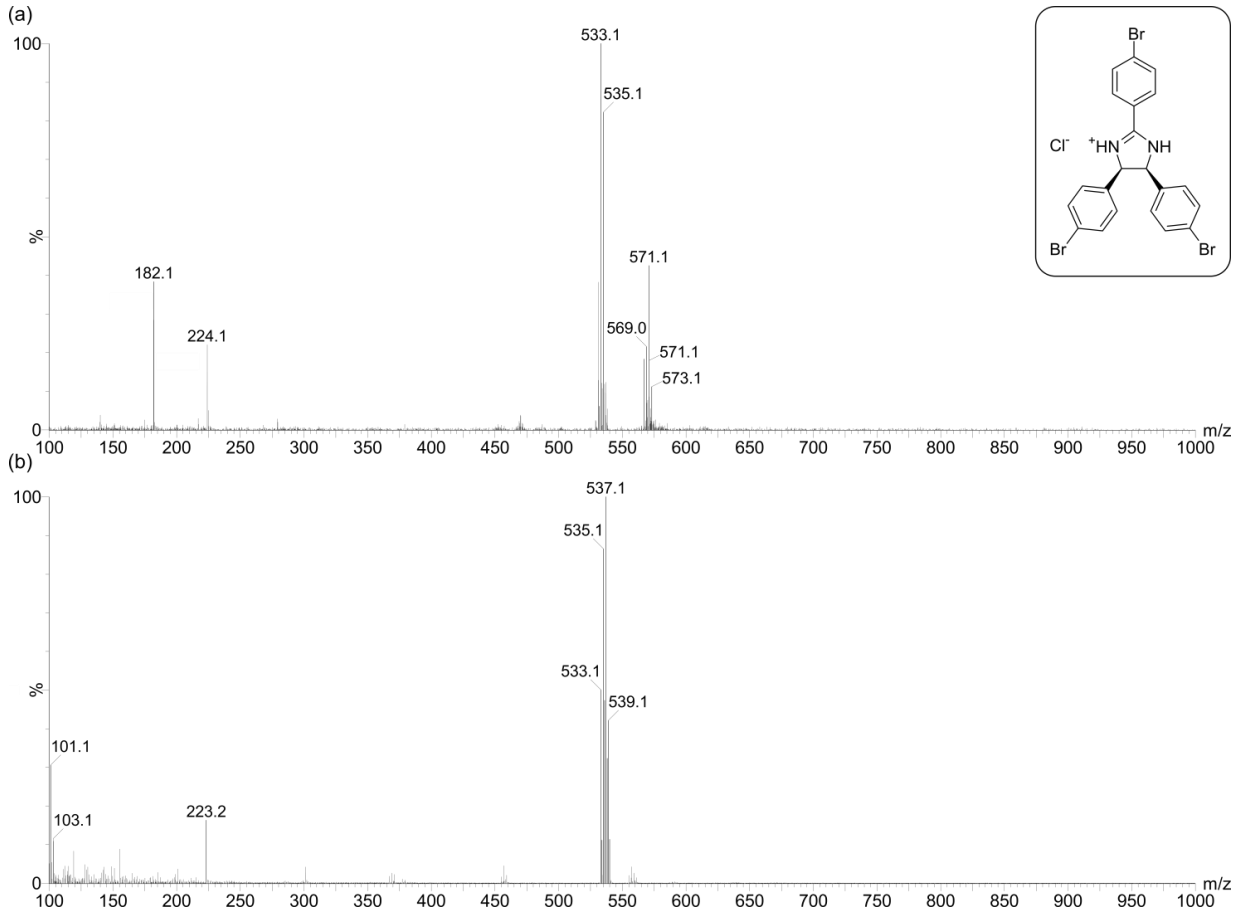


Fig. S49 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **8** with the structure in insert.

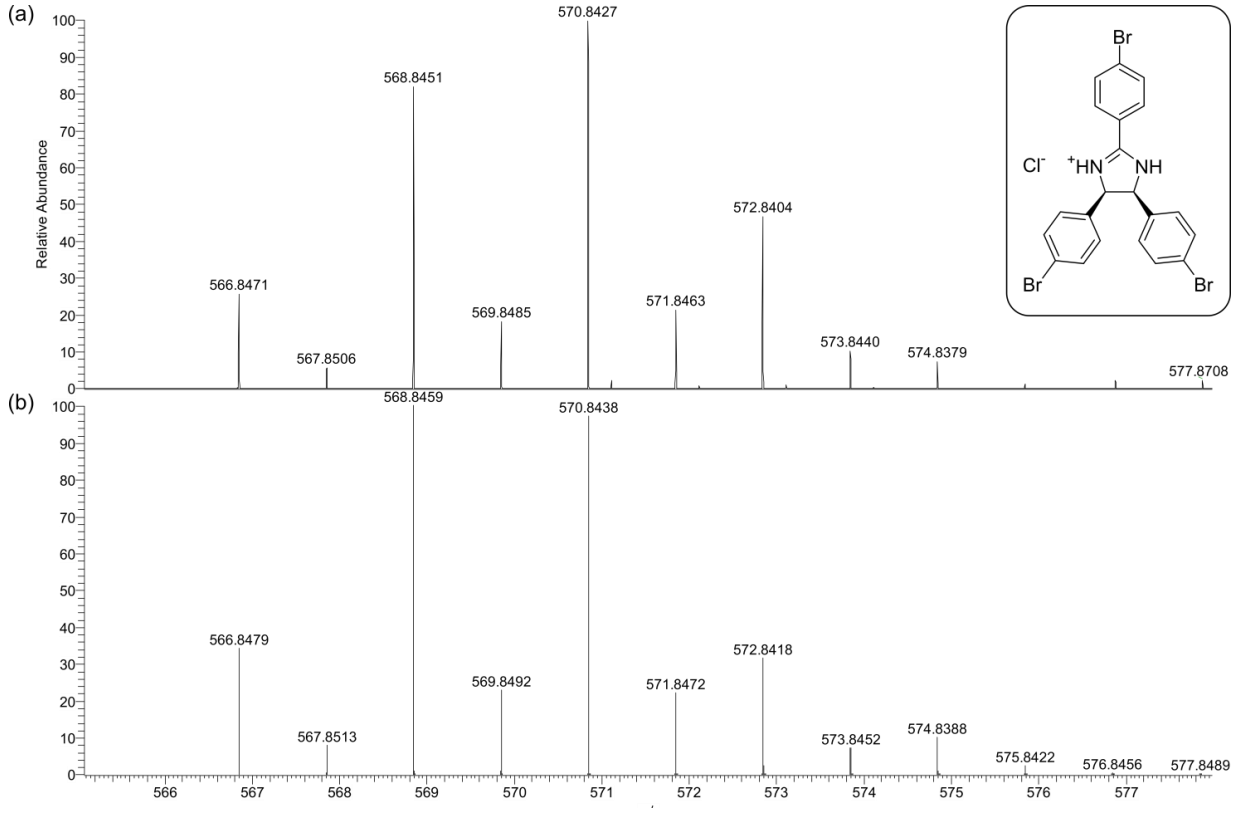


Fig. S50 (a) Observed ESI– high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+Cl]^-$ adduct with the structure of **8** in insert.

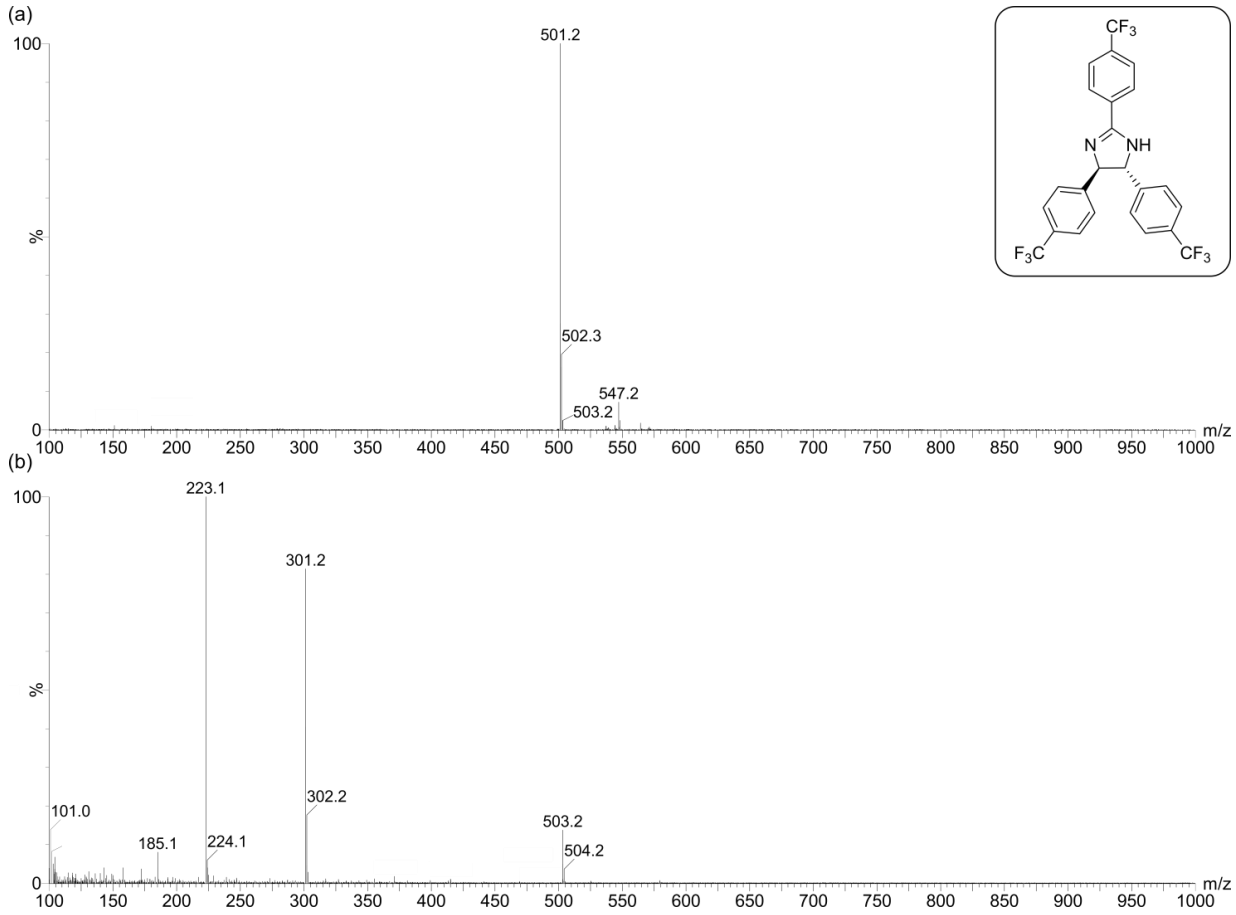


Fig. S51 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **9** with the structure in insert.

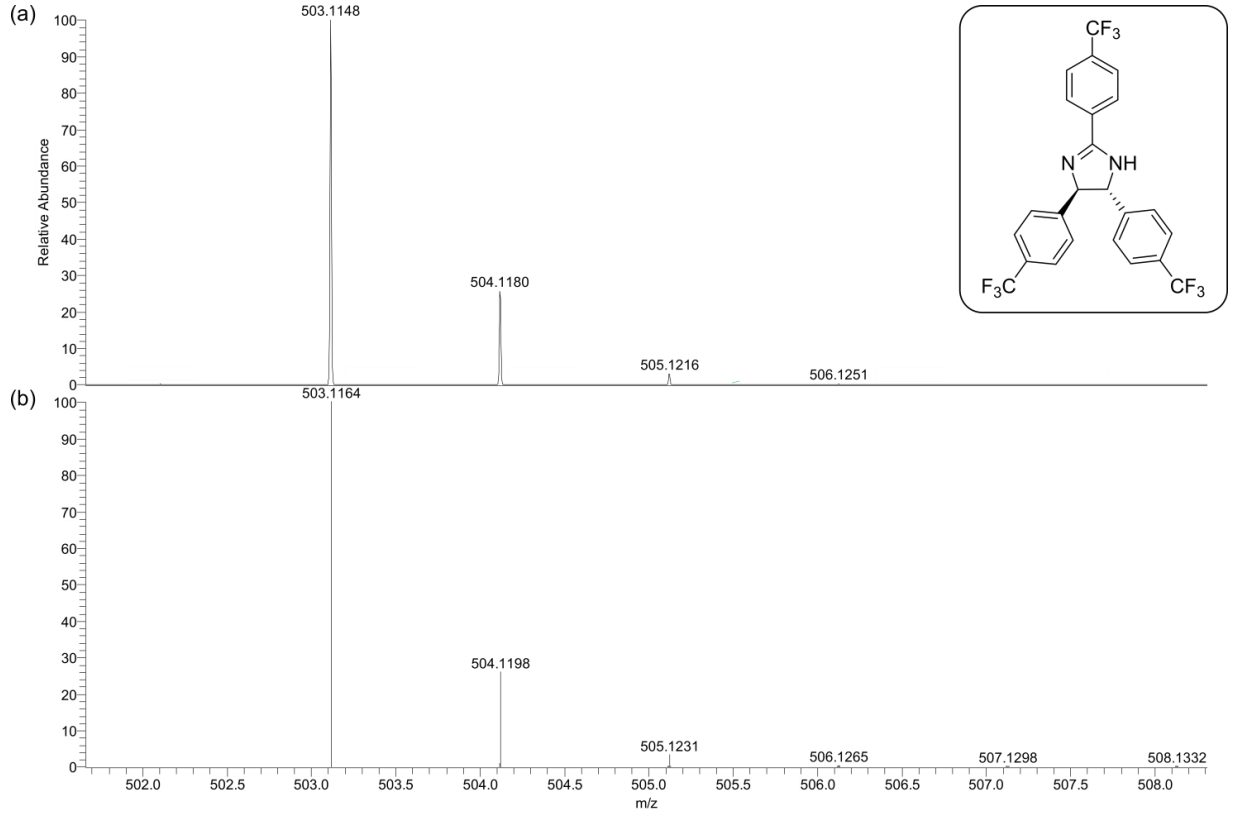


Fig. S52 (a) Observed ASAP+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **9** in insert.

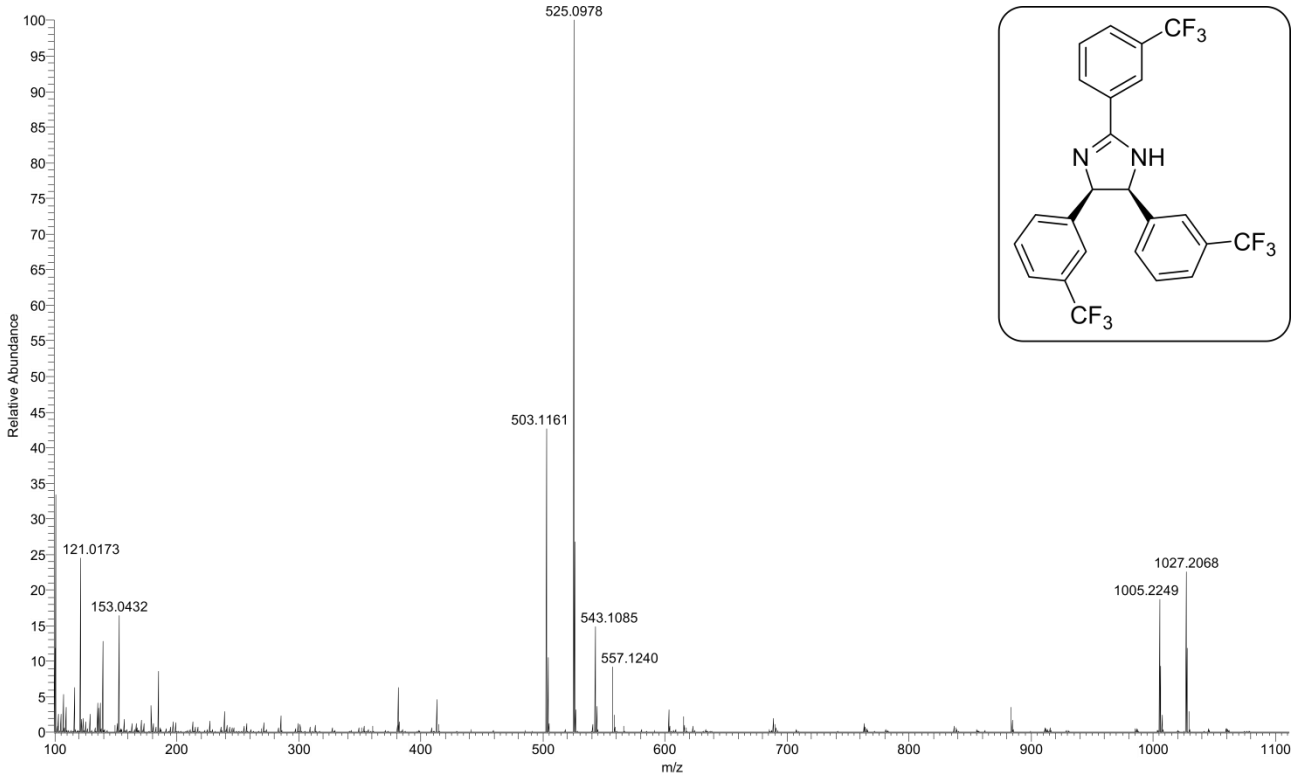


Fig. S53 ESI+/Orbitrap mass spectrum of **10** with the structure in insert.

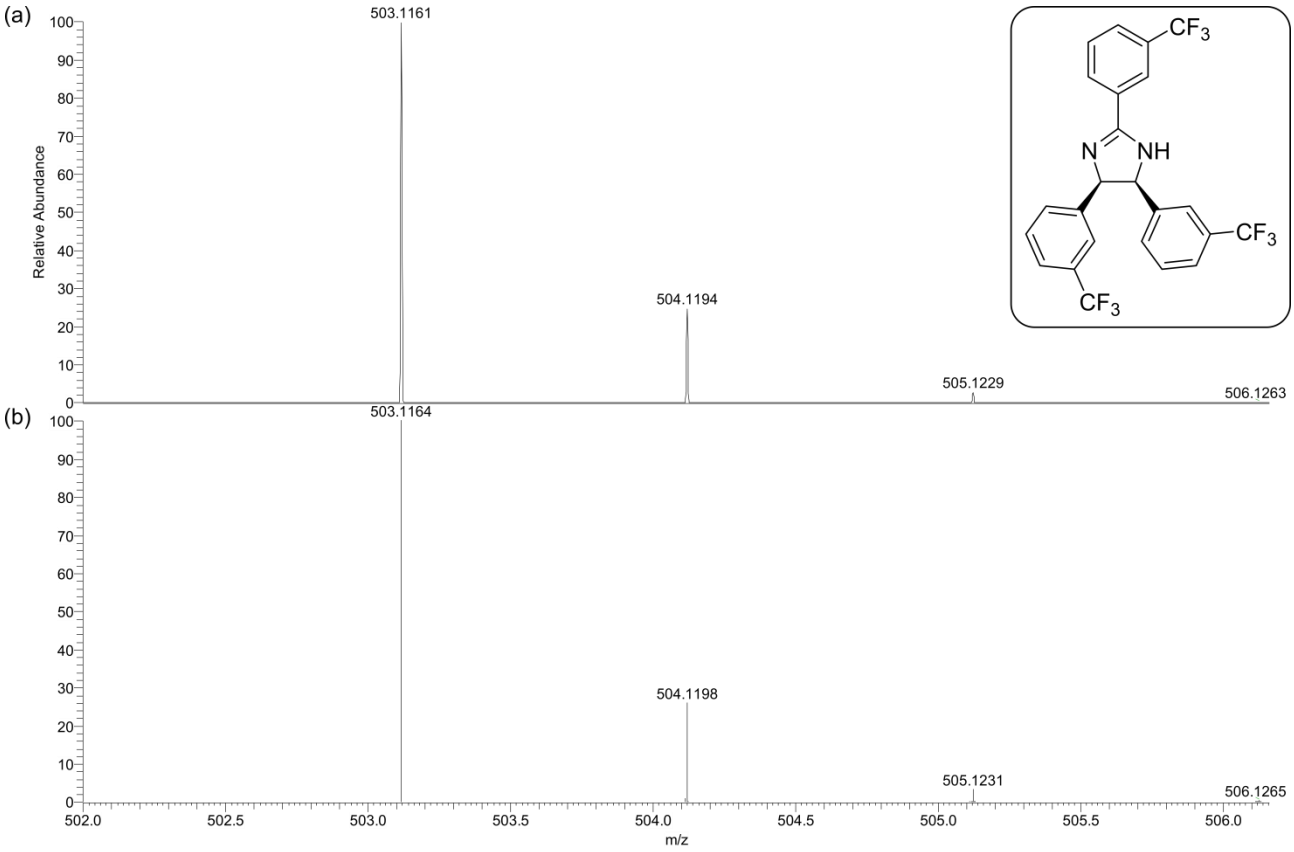


Fig. S54 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **10** in insert.

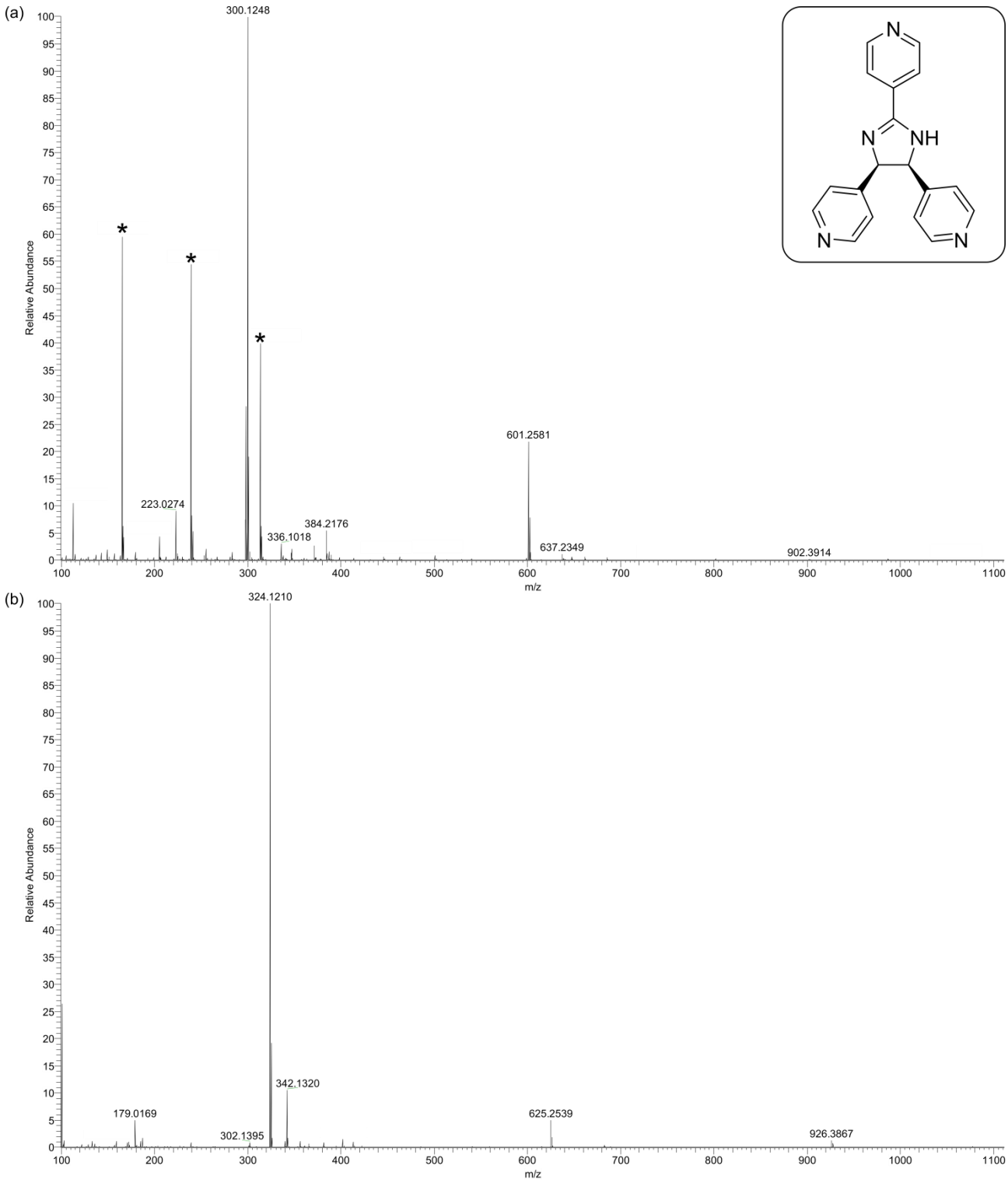


Fig. S55 (a) ESI–/Orbitrap and (b) ESI+/Orbitrap mass spectra of **11** with the structure in insert. The peaks marked with an asterix (*) are MS background peaks (m/z: 165; 239; 313).

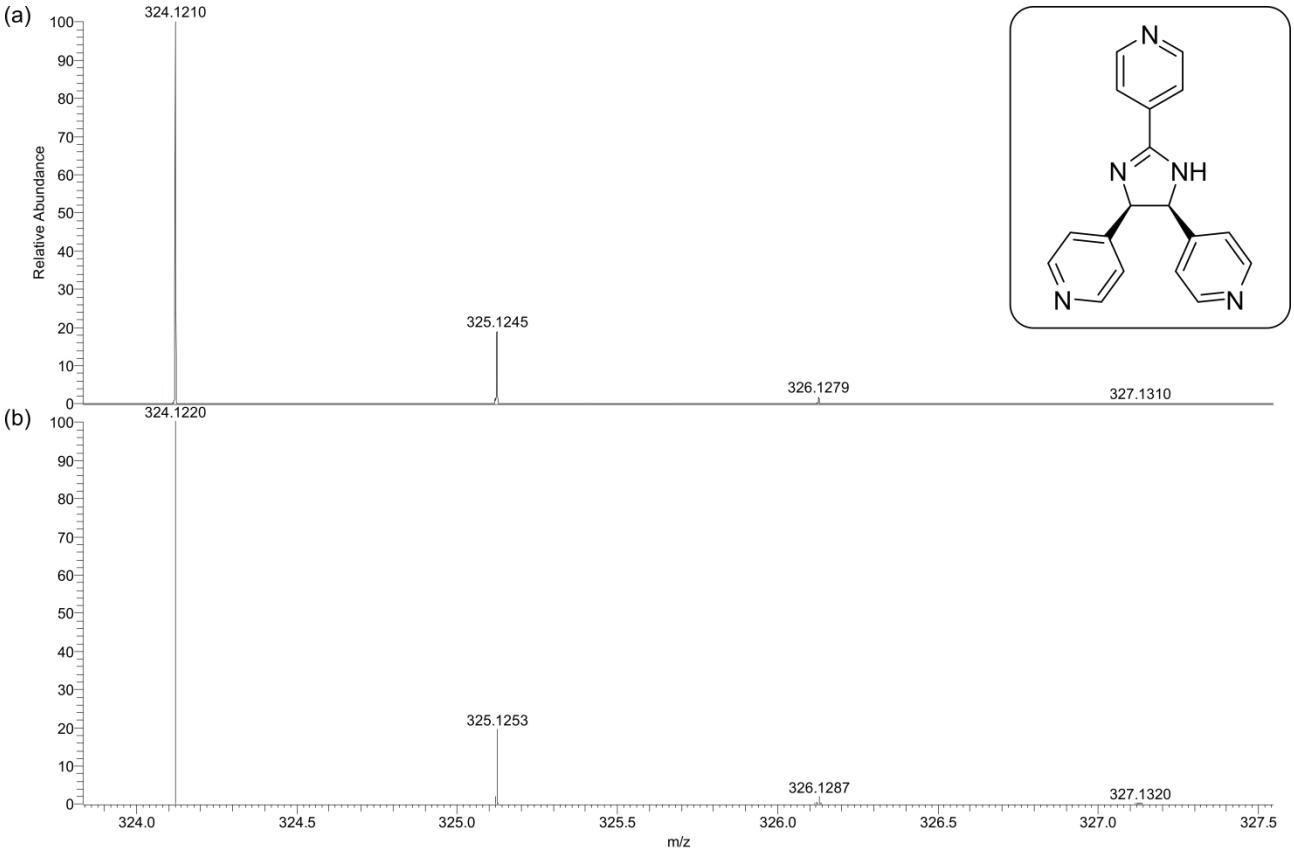


Fig. S56 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+Na]^+$ adduct with the structure of **11** in insert.

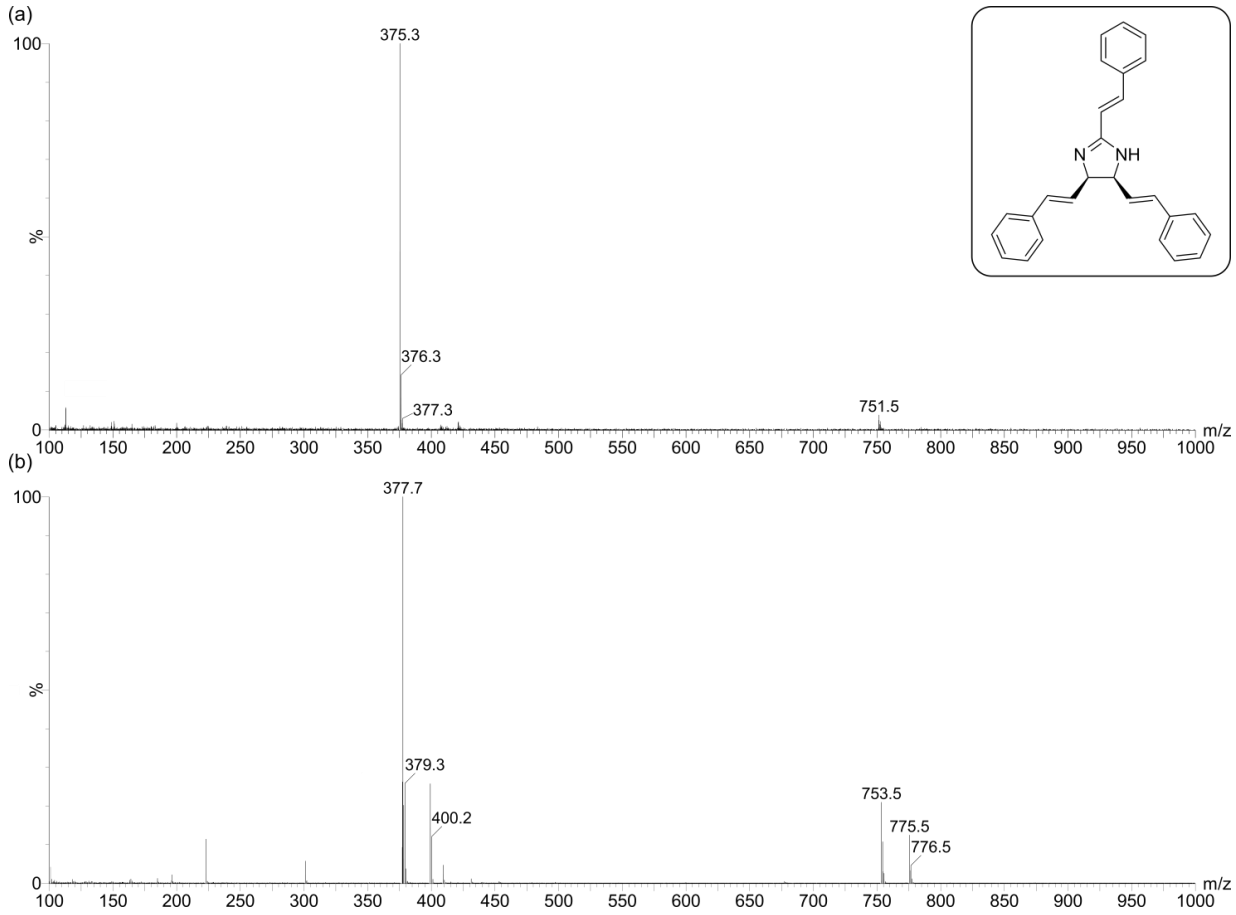


Fig. S57 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of **12** with the structure in insert.

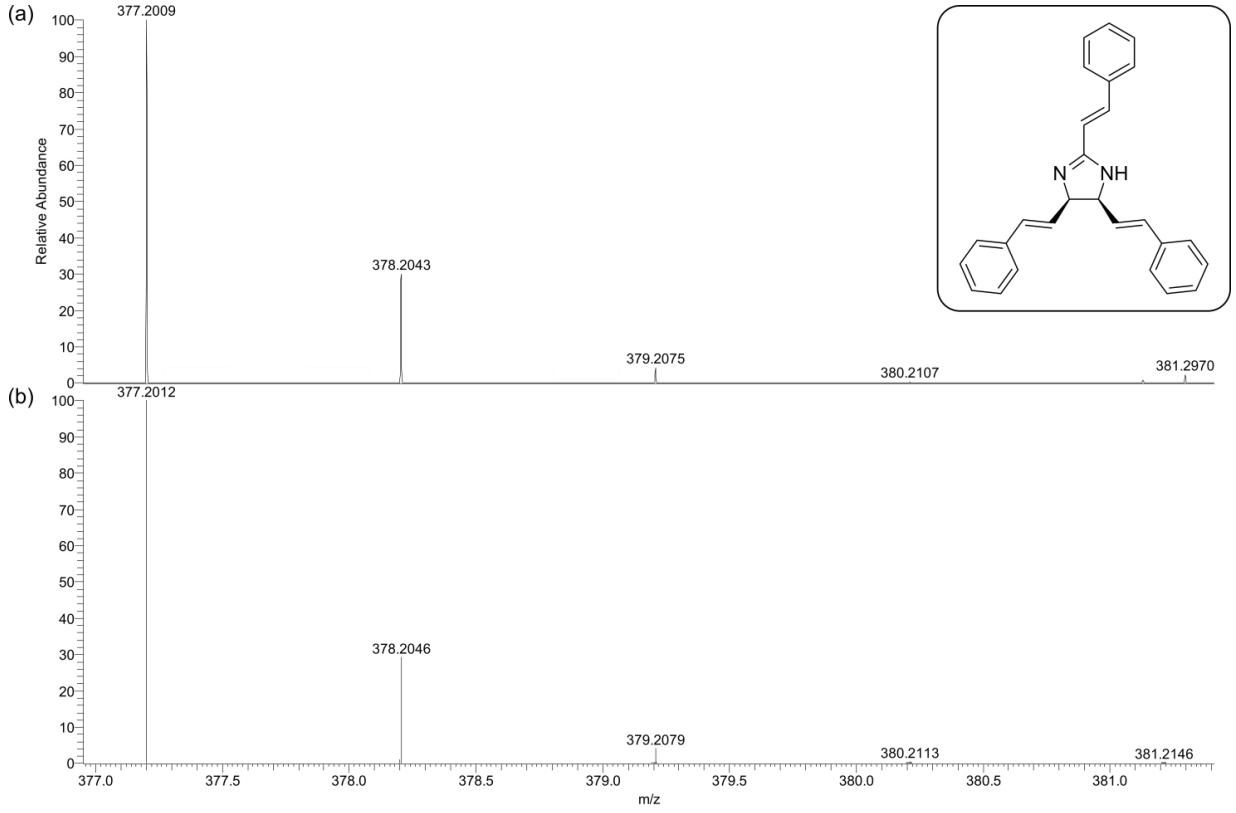


Fig. S58 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+H]^+$ ion with the structure of **12** in insert.

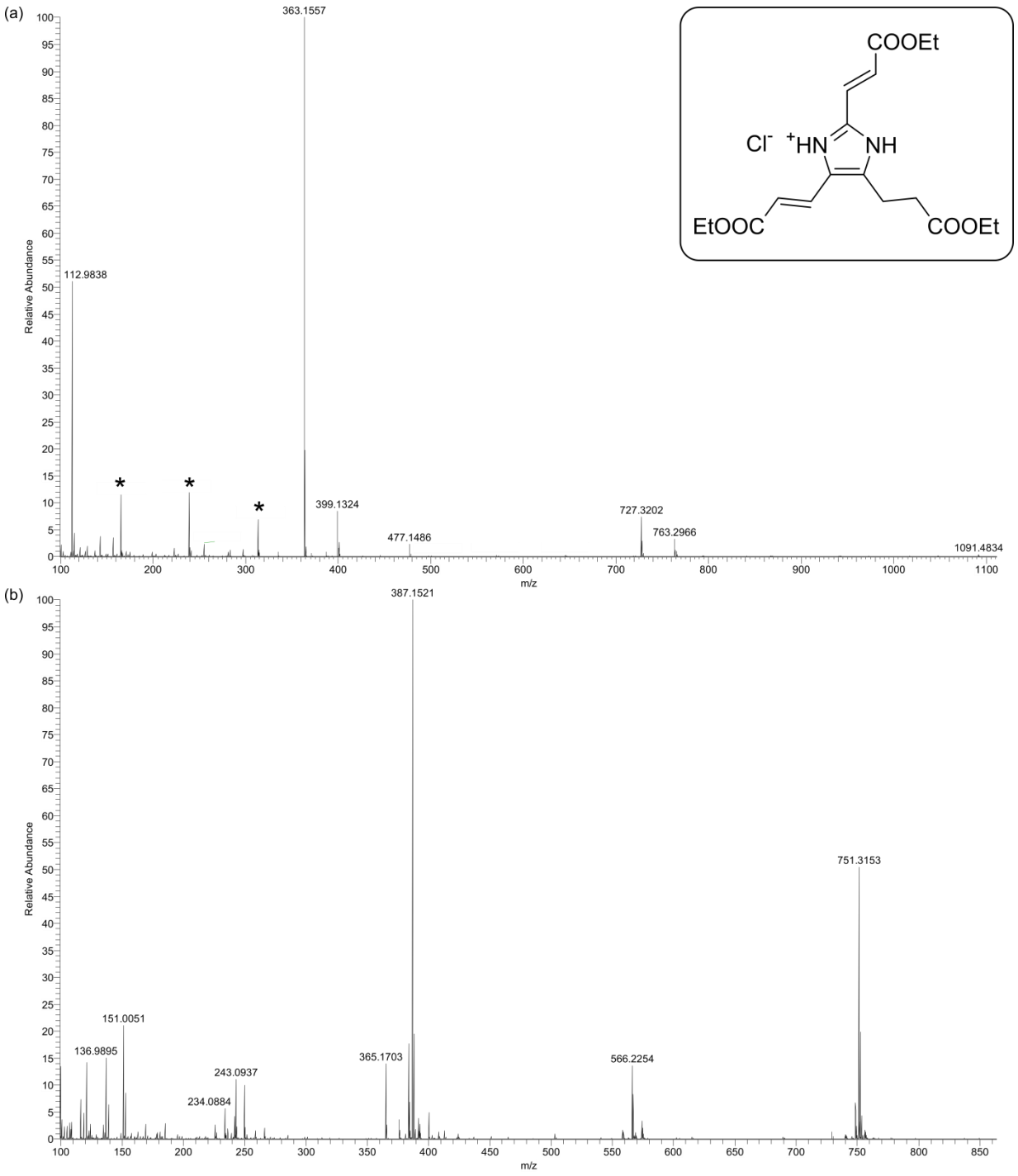


Fig. S59 (a) ESI–/Orbitrap and (b) ESI+/Orbitrap mass spectra of **13** with the structure in insert. The peaks marked with an asterix (*) are MS background peaks (m/z: 165; 239; 313).

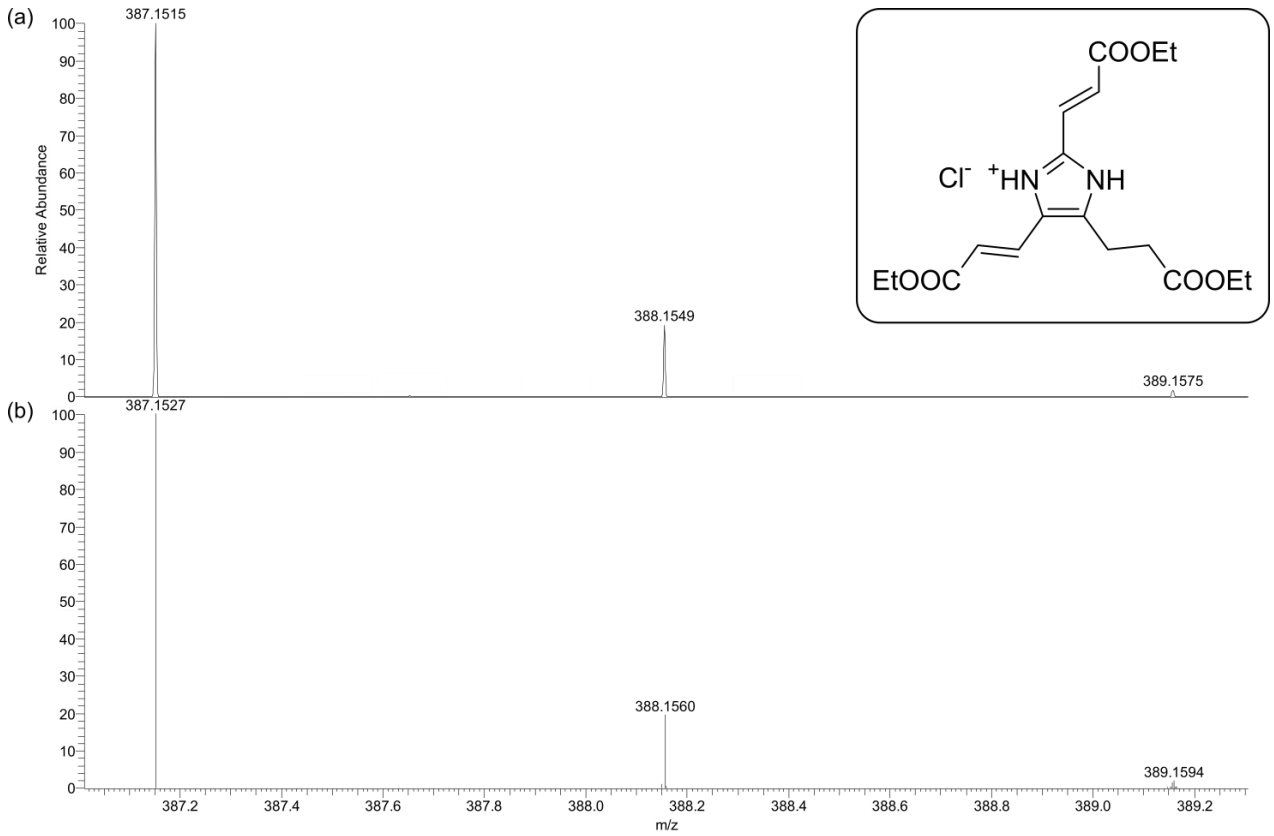


Fig. S60 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M+Na]^+$ adduct with the structure of **13** in insert.

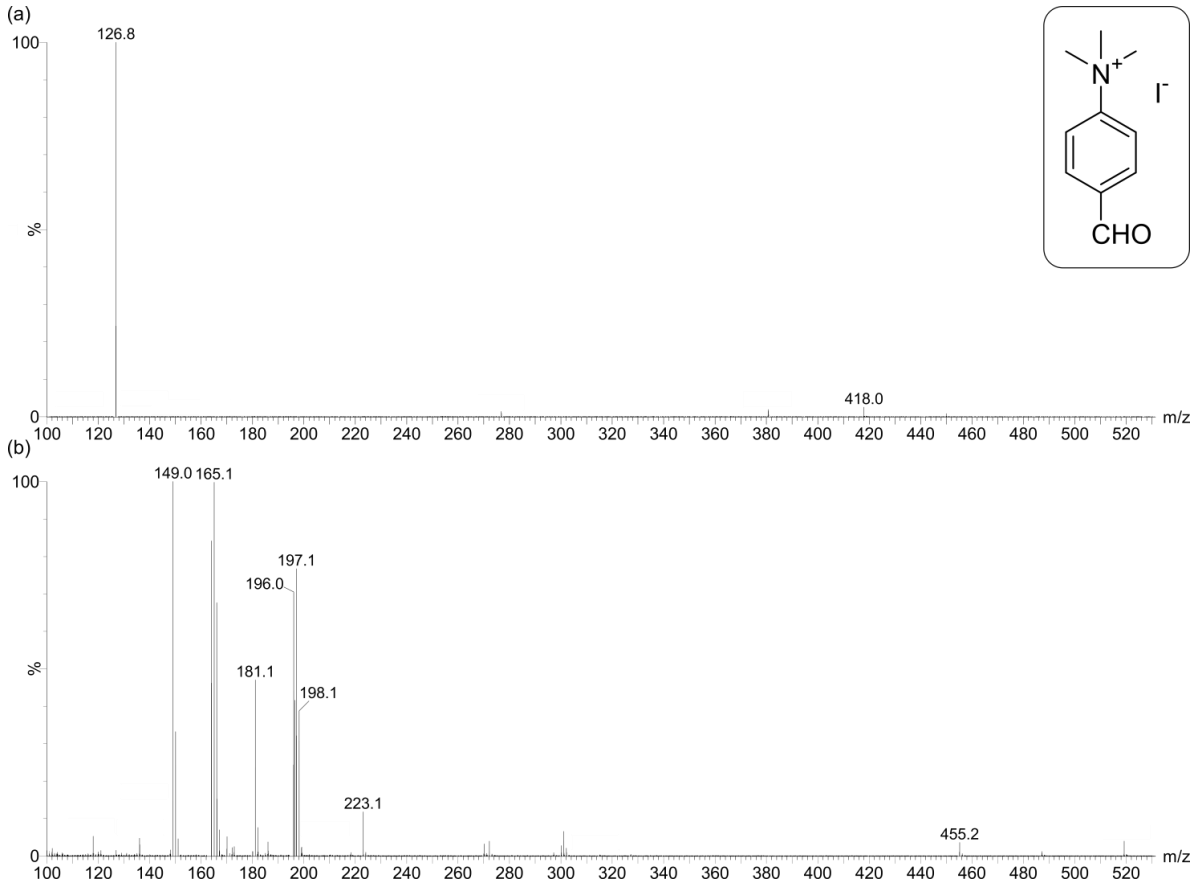


Fig. S61 (a) ESI–/SQD2 and (b) ESI+/SQD2 mass spectra of 4-formyl-*N*,*N*,*N*-trimethylanilinium iodide with the structure in insert.

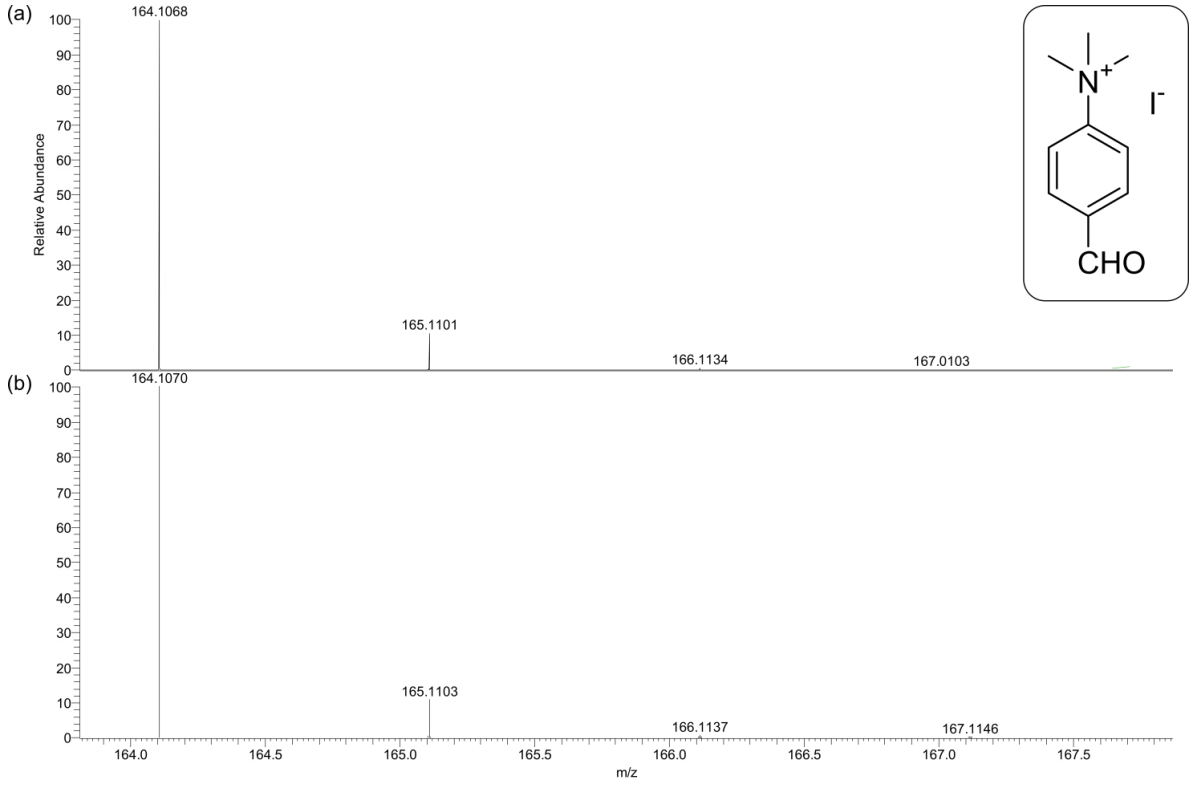
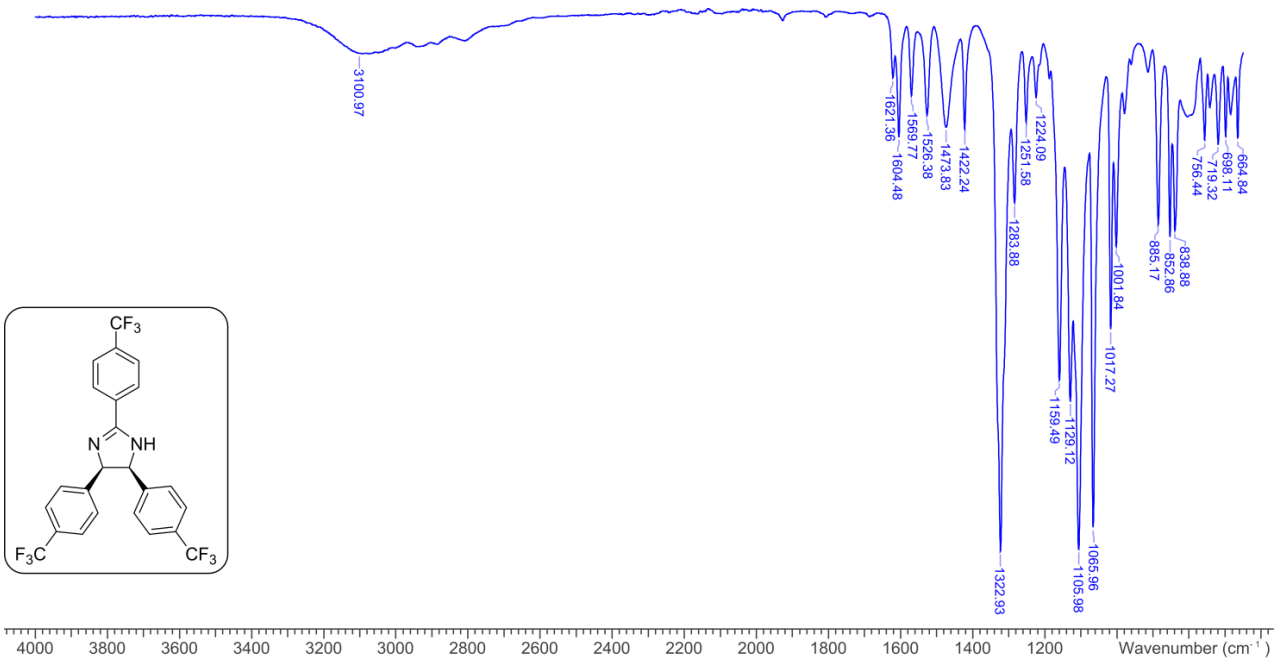


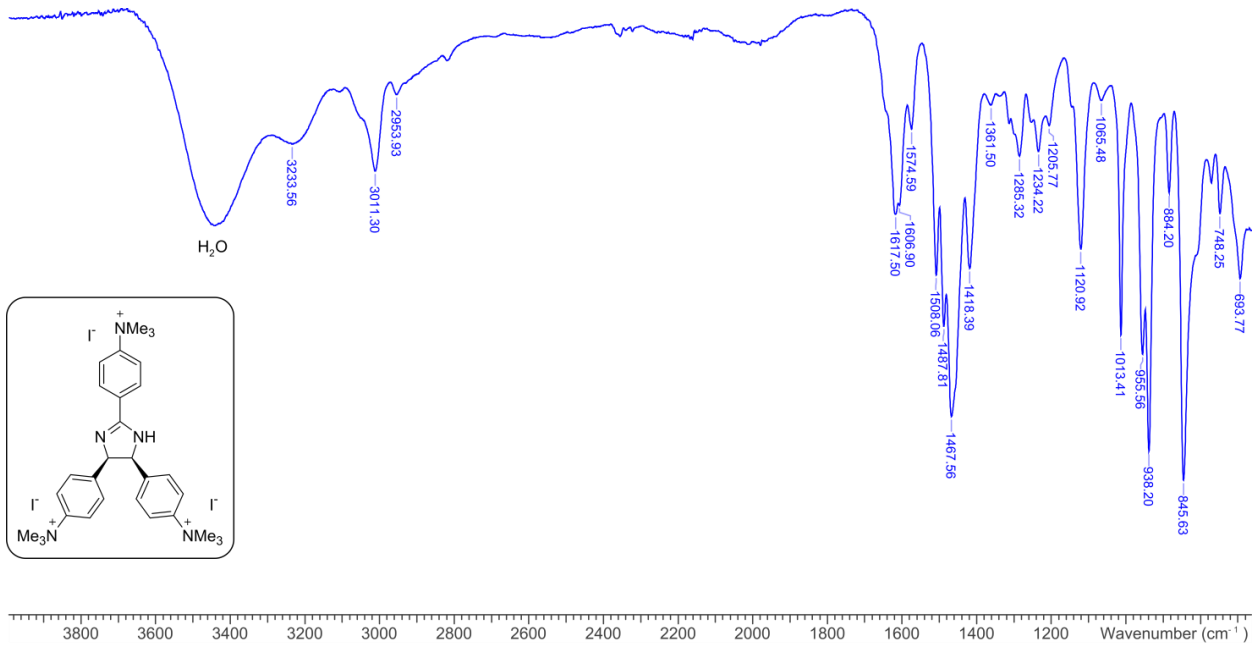
Fig. S62 (a) Observed ESI+ high resolution mass spectrum and (b) calculated isotopic distribution of the $[M]^+$ ion of 4-formyl-*N*,*N*,*N*-trimethylanilinium iodide.

4. IR spectra



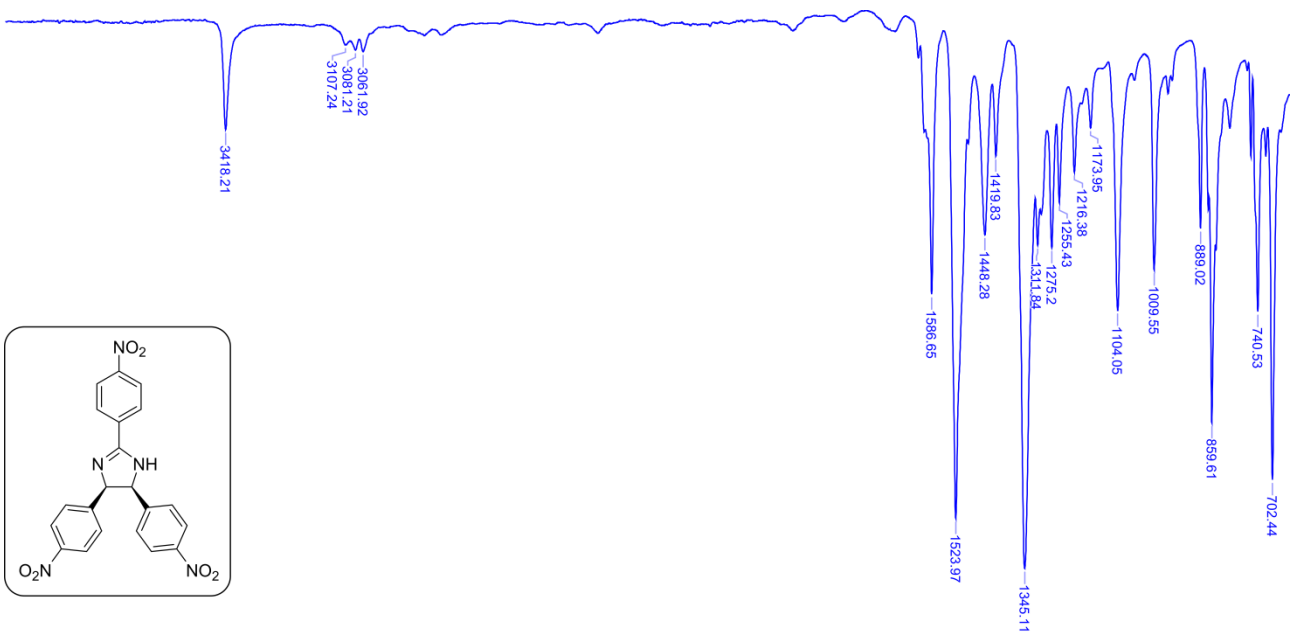
No	cm^{-1}	%T	Intensity	No	cm^{-1}	%T	Intensity	No	cm^{-1}	%T	Intensity
1	664.84	86.036	W	8	1001.84	73.389	M	15	1251.58	87.914	W
2	698.11	86.238	W	9	1017.27	63.761	M	16	1283.88	78.518	M
3	719.32	85.359	W	10	1065.96	40.624	VS	17	1322.93	37.860	VS
4	756.44	85.851	W	11	1105.98	38.063	VS	18	1422.24	87.085	W
5	838.88	75.252	M	12	1129.12	55.394	S	19	1473.83	87.344	W
6	852.86	74.539	M	13	1159.49	57.787	S	20	1526.38	88.736	W
7	885.17	75.961	M	14	1224.09	90.816	W	21	1569.77	91.017	W

Fig. S63 ATR-FTIR spectrum of **1** with the table of peaks and the structure in insert.



No	cm^{-1}	%T	Intensity	No	cm^{-1}	%T	Intensity	No	cm^{-1}	%T	Intensity
1	693.77	82.654	M	9	1120.92	84.286	M	17	1508.06	82.836	M
2	748.25	86.245	M	10	1205.77	91.093	W	18	1574.59	90.890	W
3	845.63	71.510	VS	11	1234.22	89.676	M	19	1606.90	86.707	M
4	884.20	87.377	M	12	1285.32	89.420	M	20	1617.50	86.194	M
5	938.20	73.113	VS	13	1361.50	92.235	W	21	2953.93	92.819	W
6	955.56	78.468	S	14	1418.39	83.216	M	22	3011.30	88.593	M
7	1013.41	79.535	S	15	1467.56	75.040	S	23	3233.56	90.080	W
8	1065.48	92.493	W	16	1487.81	80.014	S				

Fig. S64 ATR-FTIR spectrum of **2** with the table of peaks and the structure in insert.

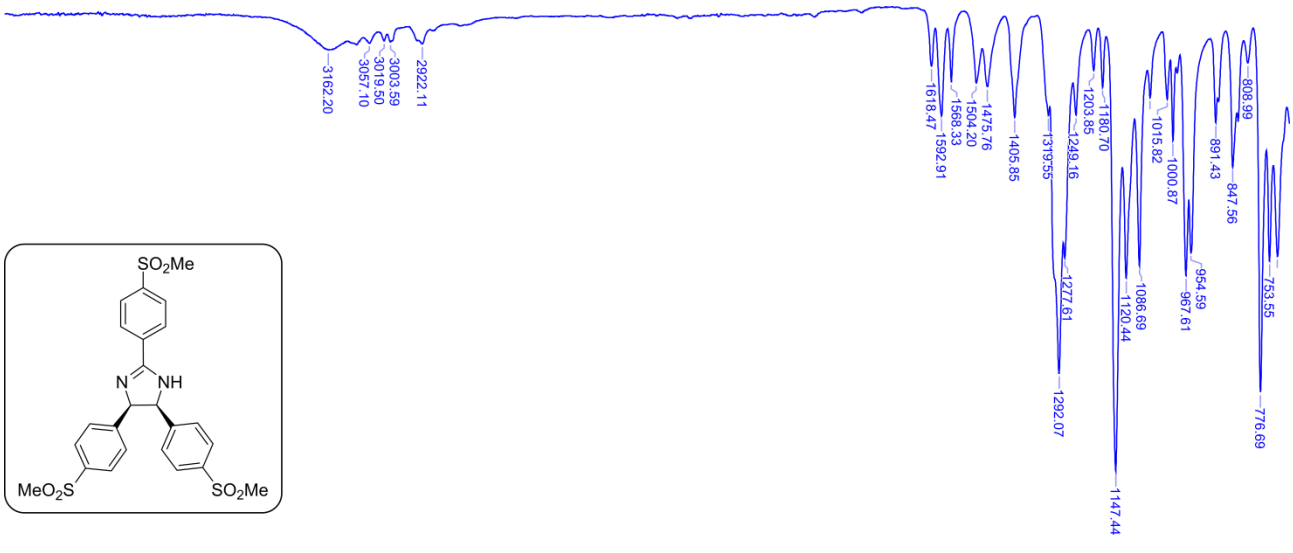


No	cm-1	%T	Intensity
1	702.44	47.728	S
2	740.53	66.129	M
3	859.61	53.968	S
4	889.02	75.224	M
5	1009.55	70.704	M
6	1104.05	66.261	M
7	1173.95	86.204	W

No	cm-1	%T	Intensity
8	1216.38	81.373	W
9	1255.43	78.000	M
10	1275.20	73.113	M
11	1311.84	73.393	M
12	1345.11	37.999	VS
13	1419.83	83.136	W
14	1448.28	74.515	M

No	cm-1	%T	Intensity
15	1523.97	43.505	VS
16	1586.65	68.036	M
17	3061.92	94.580	VW
18	3081.21	94.760	VW
19	3107.24	95.318	VW
20	3418.21	86.065	W

Fig. S65 ATR-FTIR spectrum of **3** with the table of peaks and the structure in insert.

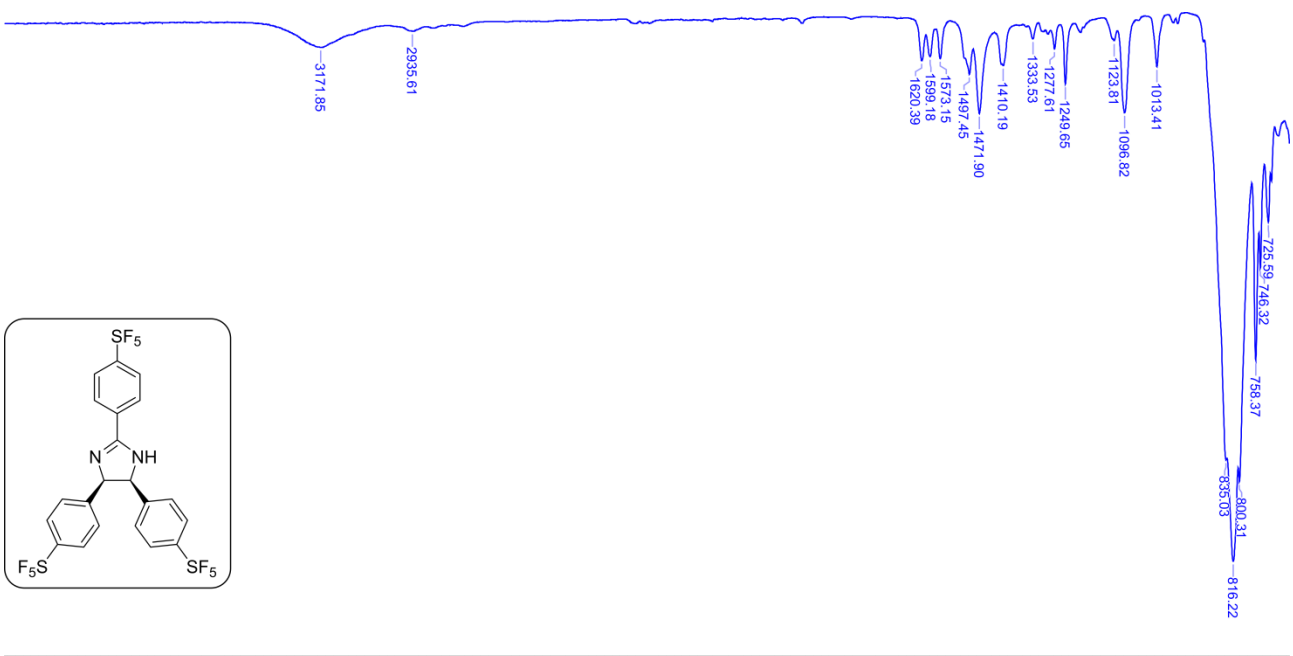


No	cm-1	%T	Intensity
1	733.30	67.290	M
2	753.55	66.714	M
3	776.69	50.369	S
4	808.99	91.453	W
5	847.56	78.443	M
6	891.43	83.975	W
7	954.59	67.740	M
8	967.61	64.904	M
9	1000.87	81.710	W
10	1015.82	86.903	W
11	1059.21	87.115	W

No	cm-1	%T	Intensity
12	1086.69	66.127	M
13	1120.44	64.605	M
14	1147.44	40.532	VS
15	1180.70	88.387	W
16	1203.85	90.514	W
17	1249.16	84.942	W
18	1277.61	67.130	M
19	1292.07	52.749	S
20	1319.55	84.888	W
21	1405.85	84.619	W
22	1475.76	88.483	W

No	cm-1	%T	Intensity
23	1504.20	88.958	W
24	1568.33	89.075	W
25	1592.91	84.862	W
26	1618.47	91.022	W
27	2922.11	93.818	VW
28	3003.59	94.049	VW
29	3019.50	94.203	VW
30	3057.10	93.878	VW
31	3162.20	93.056	VW

Fig. S66 ATR-FTIR spectrum of **4** with the table of peaks and the structure in insert.

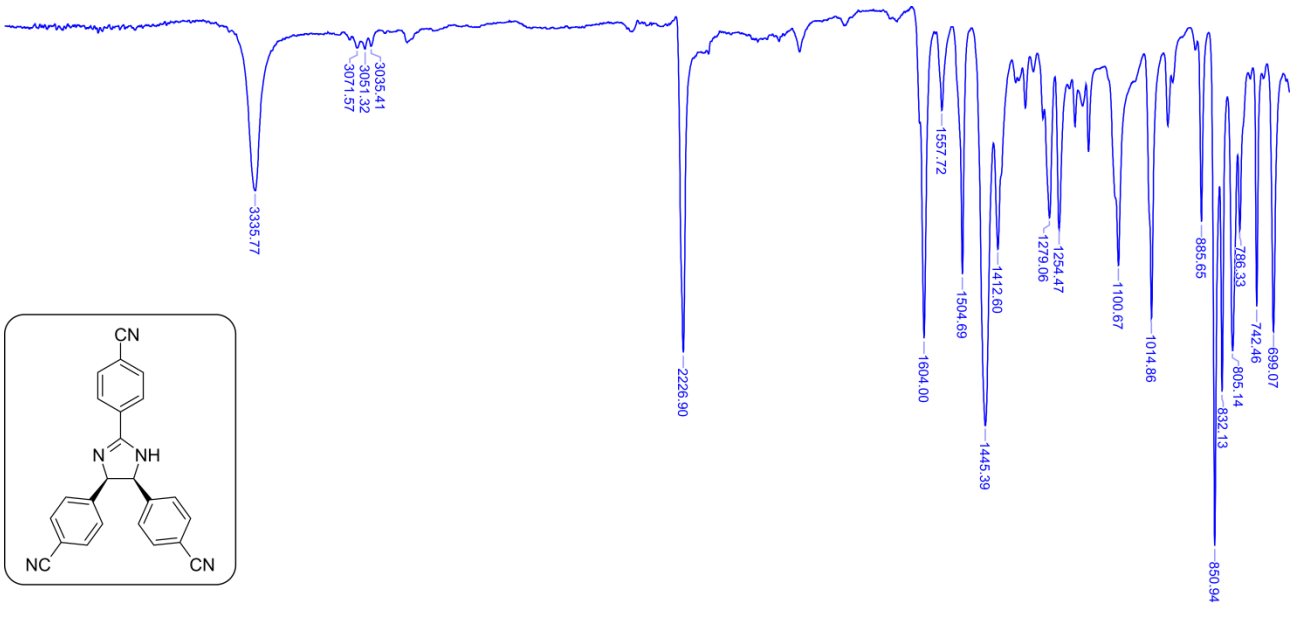


No	cm-1	%T	Intensity
1	725.59	67.112	M
2	746.32	59.711	M
3	758.37	44.969	S
4	800.31	25.501	S
5	816.22	12.709	VS
6	835.03	29.003	S
7	1013.41	92.054	VW

No	cm-1	%T	Intensity
8	1096.82	84.651	W
9	1123.81	96.231	VW
10	1249.65	89.287	W
11	1277.61	94.898	VW
12	1333.53	96.511	VW
13	1410.19	92.272	VW
14	1471.90	84.577	W

No	cm-1	%T	Intensity
15	1497.45	90.858	W
16	1573.15	93.351	VW
17	1599.18	93.694	VW
18	1620.39	93.052	VW
19	2935.61	97.785	VW
20	3171.85	95.160	VW

Fig. S67 ATR-FTIR spectrum of **5** with the table of peaks and the structure in insert.

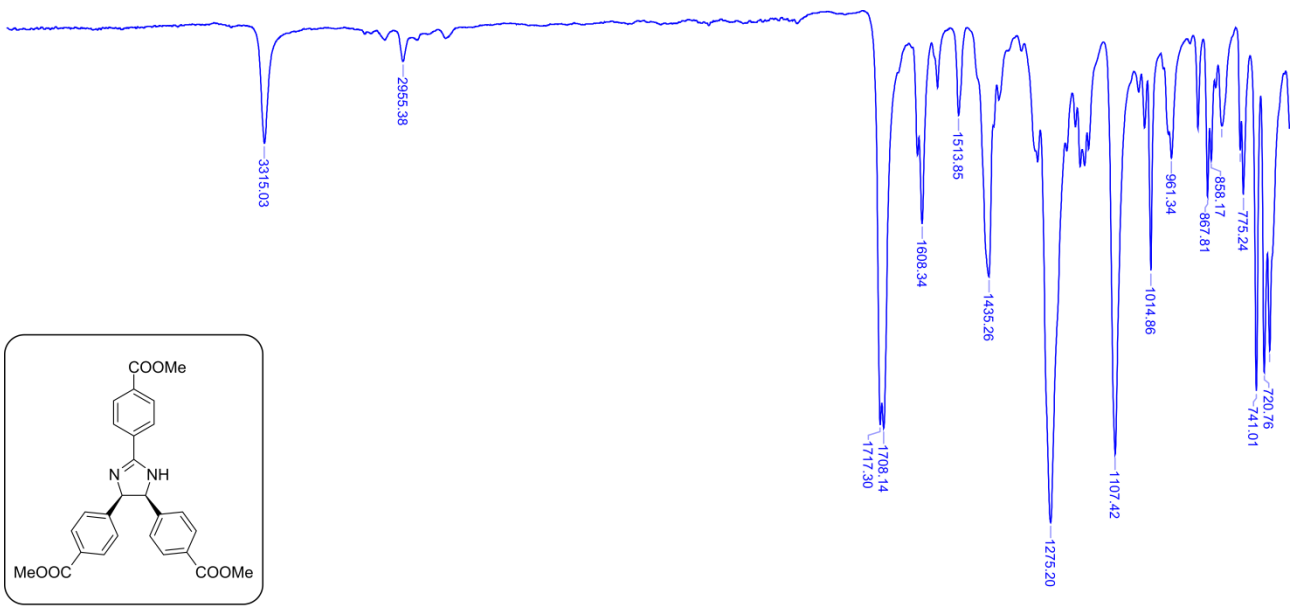


No	cm-1	%T	Intensity
1	699.07	81.064	S
2	742.46	82.378	M
3	786.33	86.382	M
4	805.14	80.066	S
5	832.13	77.917	S
6	850.94	69.829	VS
7	885.65	86.818	M

No	cm-1	%T	Intensity
8	1014.86	81.772	M
9	1100.67	84.526	M
10	1254.47	86.448	M
11	1279.06	87.036	M
12	1412.60	85.379	M
13	1445.39	76.122	S
14	1504.69	84.074	M

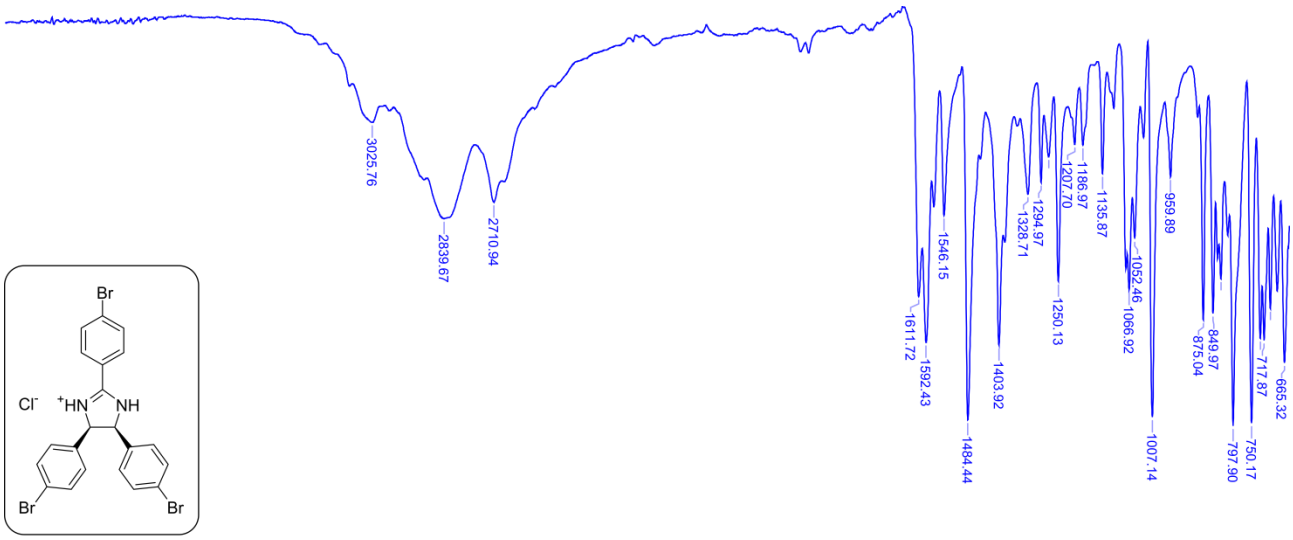
No	cm-1	%T	Intensity
15	1557.72	92.670	W
16	1604.00	80.704	S
17	2226.90	79.954	S
18	3035.41	96.031	VW
19	3051.32	95.891	VW
20	3071.57	95.938	VW
21	3335.77	88.456	M

Fig. S68 ATR-FTIR spectrum of **6** with the table of peaks and the structure in insert.



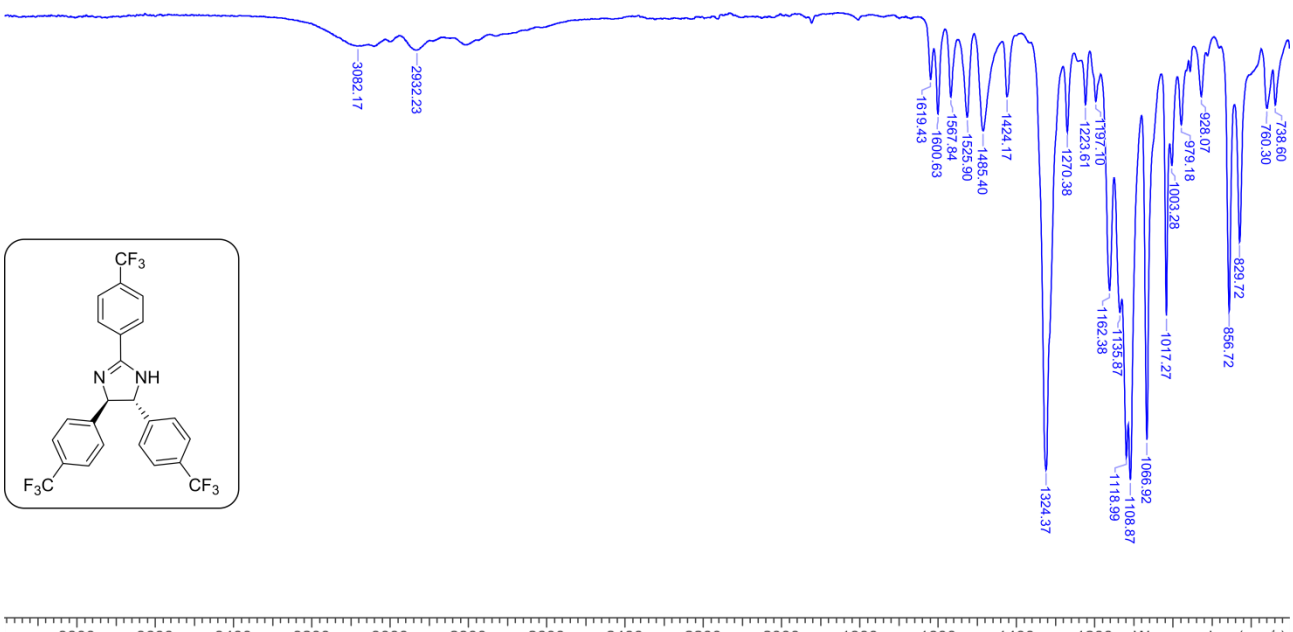
No	cm-1	%T	Intensity
1	652.30	88.650	W
2	706.78	69.346	S
3	720.76	67.327	S
4	741.01	65.599	S
5	775.24	83.793	M
6	782.96	87.931	W
7	830.69	90.198	W
8	858.17	86.976	W
9	867.81	83.634	M
10	961.34	87.211	W
11	1014.86	76.771	M
12	1107.42	59.676	S
13	1275.20	53.360	VS
14	1435.26	76.188	M
15	1513.85	91.191	W
16	1608.34	81.150	M
17	1708.14	62.108	S
18	1717.30	62.473	S
19	2955.38	96.176	VW
20	3315.03	88.583	W

Fig. S69 ATR-FTIR spectrum of **7** with the table of peaks and the structure in insert.



No	cm-1	%T	Intensity
1	665.32	70.981	S
2	701.48	74.615	S
3	717.87	72.485	S
4	727.51	72.617	S
5	750.17	66.919	VS
6	797.90	66.710	VS
7	829.24	76.634	S
8	849.97	74.308	S
9	875.04	73.863	S
10	959.89	83.507	M
11	1007.14	67.318	VS
12	1052.46	79.351	M
13	1066.92	75.902	S
14	1135.87	83.724	M
15	1186.97	85.653	M
16	1207.70	85.693	M
17	1250.13	76.475	S
18	1275.20	84.855	M
19	1294.97	83.120	M
20	1328.71	82.334	M
21	1403.92	72.152	S
22	1484.44	67.138	VS
23	1546.15	80.920	M
24	1592.43	72.343	S
25	1611.72	75.449	S
26	2710.94	81.810	M
27	2839.67	80.704	M
28	3025.76	87.179	W

Fig. S70 ATR-FTIR spectrum of **8** with the table of peaks and the structure in insert.

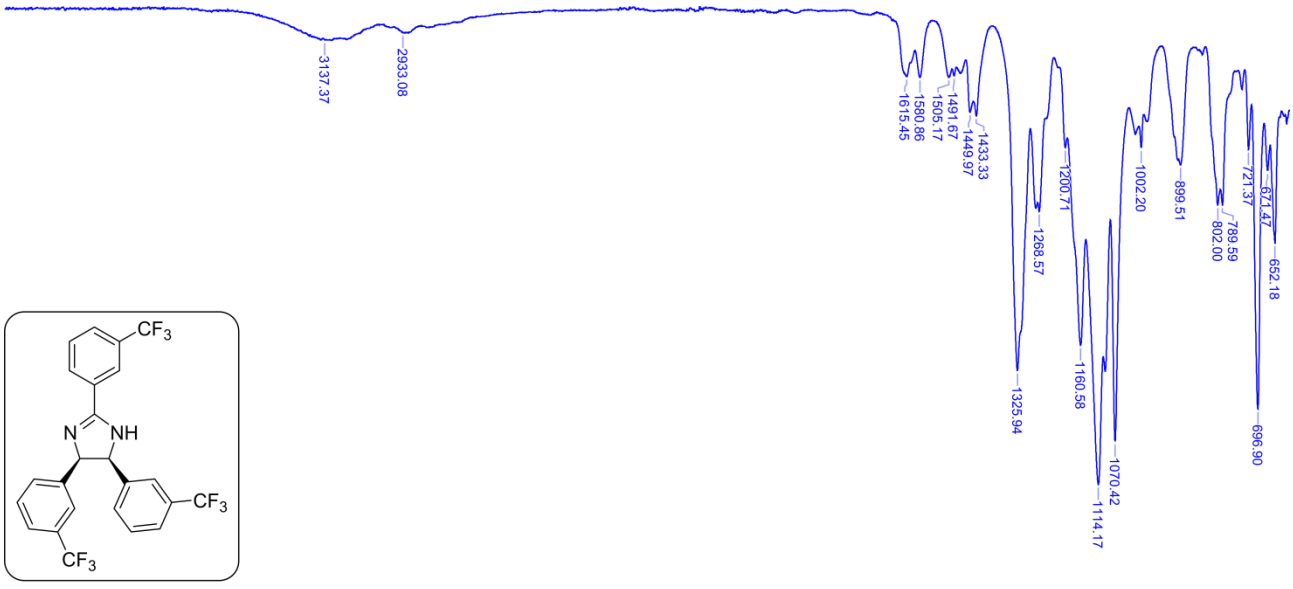


No	cm-1	%T	Intensity
1	738.60	88.534	W
2	760.30	88.049	W
3	829.72	68.744	M
4	856.72	58.787	S
5	928.07	89.770	W
6	979.18	85.707	W
7	1003.28	79.838	M
8	1017.27	58.147	S
9	1066.92	40.224	VS

No	cm-1	%T	Intensity
10	1108.87	34.400	VS
11	1118.99	37.707	VS
12	1135.87	58.588	S
13	1162.38	61.779	M
14	1197.10	89.046	W
15	1223.61	88.608	W
16	1270.38	84.664	W
17	1324.37	35.863	VS
18	1424.17	89.729	W

No	cm-1	%T	Intensity
19	1485.40	84.807	W
20	1525.90	86.786	W
21	1567.84	89.701	W
22	1600.63	87.235	W
23	1619.43	92.246	W
24	2932.23	96.459	VW
25	3082.17	97.061	VW

Fig. S71 ATR-FTIR spectrum of **9** with the table of peaks and the structure in insert.

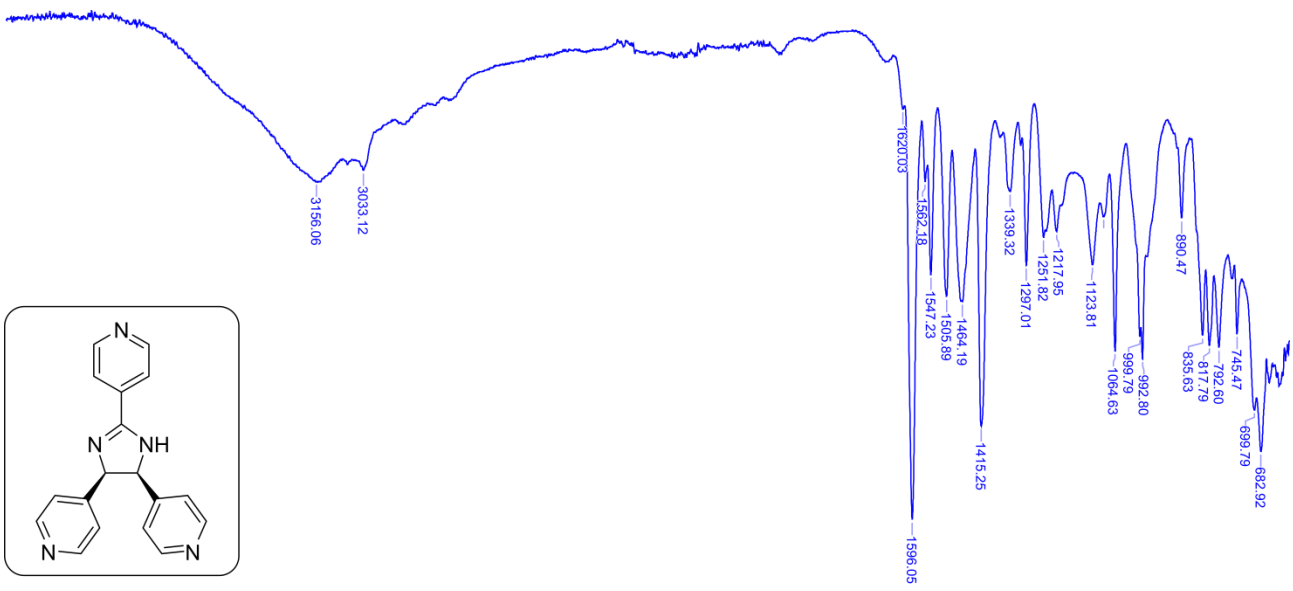


No	cm-1	%T	Intensity
1	652.18	61.833	M
2	671.47	73.984	M
3	696.90	34.068	S
4	721.37	77.550	M
5	789.59	68.216	M
6	802.00	68.211	M
7	899.51	74.974	M
8	1002.20	77.777	M

No	cm-1	%T	Intensity
9	1070.42	28.647	VS
10	1114.17	21.475	VS
11	1160.58	44.790	S
12	1200.71	77.857	M
13	1268.57	67.172	M
14	1325.94	40.527	S
15	1433.33	83.189	W
16	1449.97	83.776	W

No	cm-1	%T	Intensity
17	1491.67	89.900	W
18	1505.17	89.604	W
19	1580.86	89.601	W
20	1615.45	89.734	W
21	2933.08	97.088	W
22	3137.37	95.889	W

Fig. S72 ATR-FTIR spectrum of **10** with the table of peaks and the structure in insert.

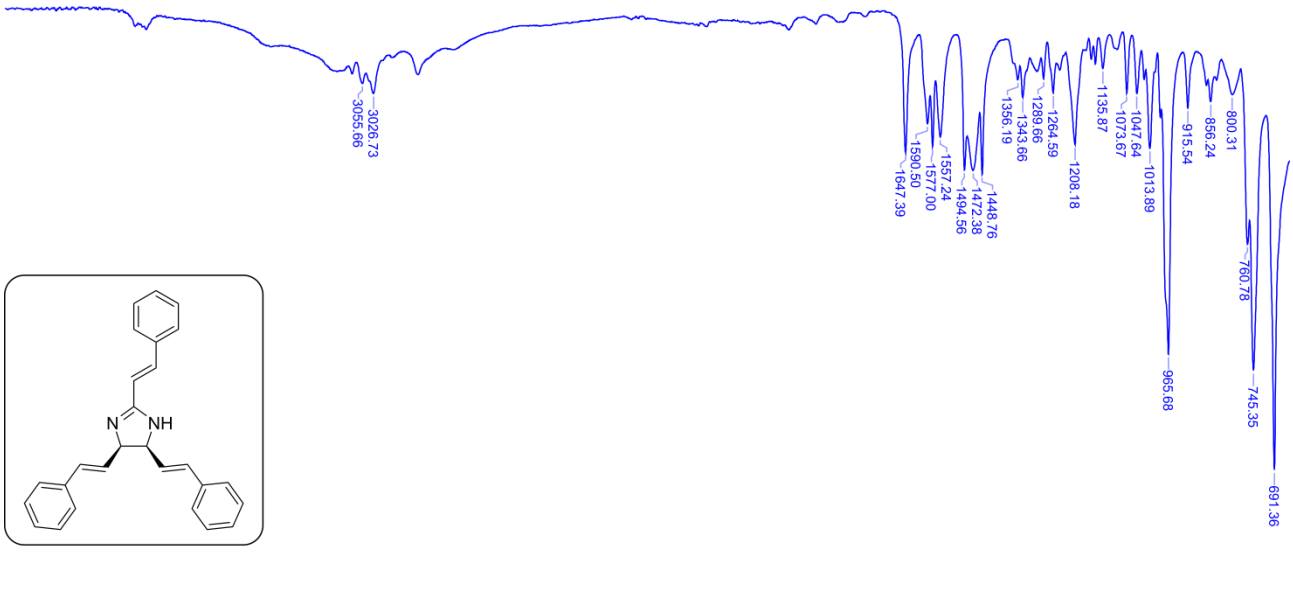


No	cm⁻¹	%T	Intensity
1	682.92	68.751	M
2	699.79	71.533	M
3	745.47	76.644	M
4	792.60	75.713	M
5	817.79	75.865	M
6	835.63	76.518	M
7	890.47	84.388	M
8	992.80	74.966	M
9	999.79	76.435	M

No	cm⁻¹	%T	Intensity
10	1064.63	75.482	M
11	1094.89	84.485	M
12	1123.81	81.275	M
13	1217.95	83.506	M
14	1251.82	83.117	M
15	1297.01	81.237	M
16	1339.32	86.197	W
17	1415.25	70.457	M
18	1464.19	78.801	M

No	cm⁻¹	%T	Intensity
19	1505.89	79.143	M
20	1547.23	80.605	M
21	1562.18	86.862	W
22	1596.05	64.194	S
23	1620.03	91.708	W
24	3033.12	87.596	W
25	3156.06	86.852	W

Fig. S73 ATR-FTIR spectrum of **11** with the table of peaks and the structure in insert.

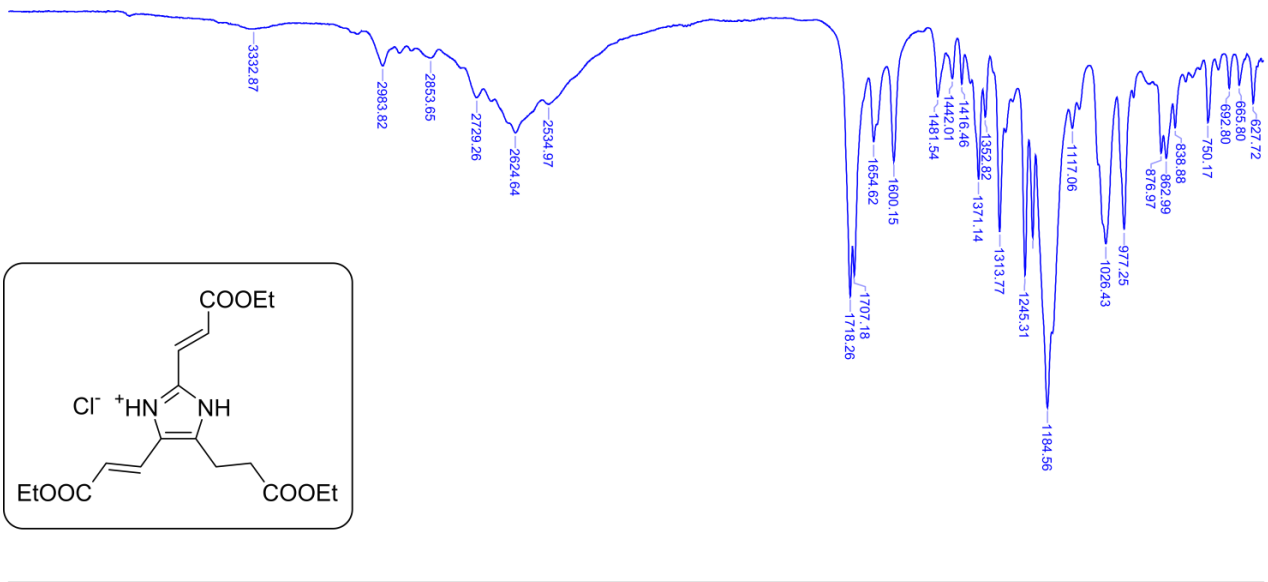


No	cm⁻¹	%T	Intensity
1	691.36	43.989	VS
2	745.35	55.314	S
3	760.78	69.706	M
4	800.31	86.750	W
5	856.24	85.946	W
6	915.54	85.210	W
7	965.68	57.153	S
8	1013.89	80.617	M
9	1047.64	86.882	W

No	cm⁻¹	%T	Intensity
10	1073.67	86.885	W
11	1135.87	89.728	W
12	1208.18	81.072	W
13	1264.59	86.933	W
14	1289.66	88.531	W
15	1343.66	86.430	W
16	1356.19	88.444	W
17	1448.76	77.665	M
18	1472.38	78.120	M

No	cm⁻¹	%T	Intensity
19	1494.56	78.145	M
20	1557.24	81.946	W
21	1577.00	80.822	M
22	1590.50	83.430	W
23	1647.39	80.150	M
24	3026.73	86.873	W
25	3055.66	88.014	W

Fig. S74 ATR-FTIR spectrum of **12** with the table of peaks and the structure in insert.

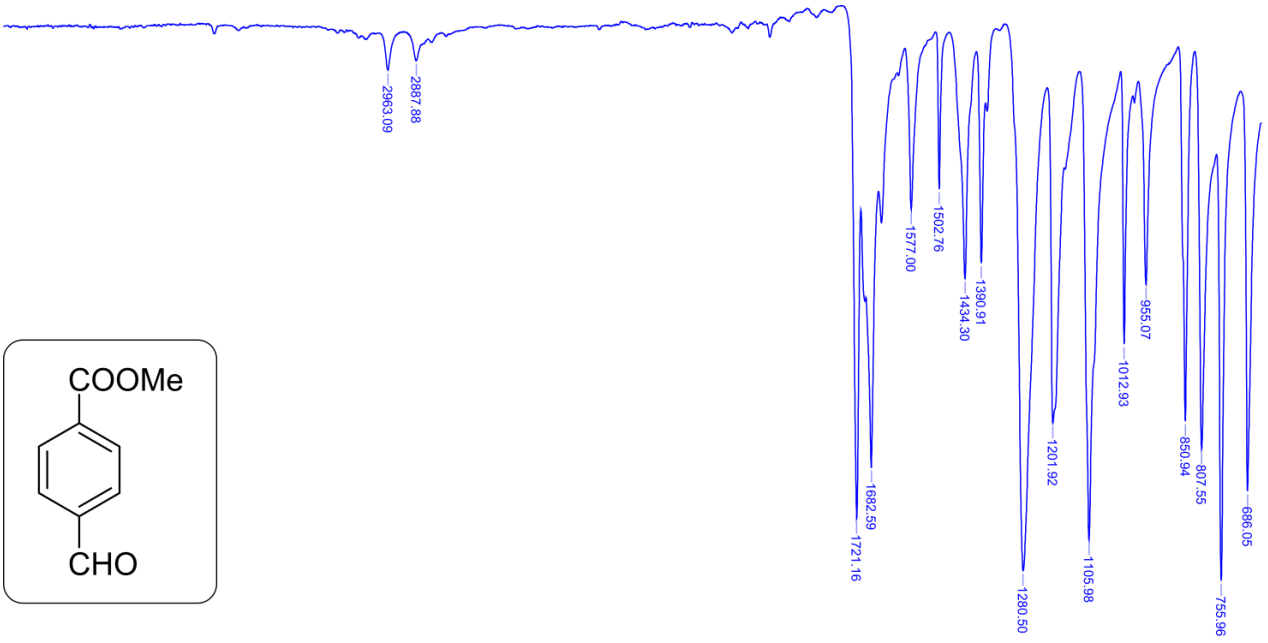


No	cm⁻¹	%T	Intensity
1	627.72	83.309	W
2	665.80	86.569	W
3	692.80	85.997	W
4	750.17	79.871	W
5	838.88	78.931	W
6	862.99	73.453	M
7	876.97	74.412	M
8	977.25	60.659	M
9	1026.43	58.140	M
10	1117.06	78.907	W

No	cm⁻¹	%T	Intensity
11	1184.56	28.749	VS
12	1224.58	59.299	M
13	1245.31	52.441	S
14	1313.77	60.357	M
15	1352.82	80.856	W
16	1371.14	69.742	M
17	1416.46	86.758	W
18	1442.01	87.774	W
19	1481.54	84.504	W
20	1600.15	72.867	M

No	cm⁻¹	%T	Intensity
21	1654.62	76.471	M
22	1707.18	52.372	S
23	1718.26	48.676	S
24	2534.97	83.181	W
25	2624.64	78.035	M
26	2729.26	84.362	W
27	2853.65	91.480	W
28	2983.82	90.060	W
29	3332.87	96.700	VW

Fig. S75 ATR-FTIR spectrum of **13** with the table of peaks and the structure in insert.



No	cm⁻¹	%T	Intensity
1	686.05	55.304	S
2	755.96	47.289	VS
3	807.55	59.093	S
4	850.94	61.604	S
5	955.07	73.862	M
6	1012.93	68.508	M

No	cm⁻¹	%T	Intensity
7	1105.98	50.928	VS
8	1201.92	61.411	S
9	1280.50	48.193	VS
10	1390.91	75.781	M
11	1434.30	74.407	M
12	1502.76	82.397	M

No	cm⁻¹	%T	Intensity
13	1577.00	80.617	M
14	1682.59	57.468	S
15	1721.16	52.855	S
16	2887.88	93.940	VW
17	2963.09	93.094	W

Fig. S76 ATR-FTIR spectrum of methyl 4-formylbenzoate with the table of peaks and the structure in insert.

5. HPLC analysis

5.1. HPLC methods

When necessary, preparative HPLC was used for the purification in order to obtain high purity products (>99%). For the preparative HPLC purification VWR LaPrep Sigma instrument was used with preparative solvent pump (La Prep Sigma LP1200), sample injection pump (La Prep Sigma LP1000), UV detector (La Prep Sigma LP3101), Interchim, Uptisphere Strategy 100A, 10 µm, C18-3 (250 × 30 mm) column; with eluent A: water type I (18.2 MΩ) with 0.1% TFA and eluent B: methanol.

For Methods 1–4, HPLC analyses were performed on an ACE-C18, 5 µm, 100 Å, 150 × 4.6 mm column from Hichrom. The solvent system used was: eluent A: water type I (18.2 MΩ) with 0.1 % TFA and eluent B: acetonitrile with 0.1% TFA. Gradient elution was selected with 1 mL min^{-1} flow rate, detection at 250 nm and column temperature at 30 °C.

For Method 5, HPLC analyses were performed on a SeQuant® ZIC®-HILIC, 5 µm, 200 Å, 150 × 4.6 mm column from Merck. The solvent system used was eluent A: Triethyl ammonium acetate (100 mM) buffer and eluent B: acetonitrile with triethyl ammonium acetate (10 mM). Gradient elution was selected with 0.7 mL min^{-1} flow rate, detection at 250 nm or 280 nm and column temperature at 30 °C.

Method 1

The separation of compounds was achieved with 0.1% TFA in water and 0.1% TFA in acetonitrile gradient elution. B was held at 50% for 3 min, and then was eluted from 50% to 75% in 9 min.

Method 2

The separation of compounds was achieved with 0.1% TFA in water and 0.1% TFA in acetonitrile gradient elution. B was held at 25% for 3 min, and then was eluted from 25% to 50% in 11 min.

Method 3

The separation of compounds was achieved with 0.1% TFA in water and 0.1% TFA in acetonitrile gradient elution B was held at 10% for 3 min, and then was eluted from 10% to 50% in 9 min.

Method 4

The separation of compounds was achieved with 0.1 % TFA in water and 0.1 % TFA in acetonitrile gradient elution. B was held at 5% for 3 min then was eluted from 5% to 80% in 11 min.

Method 5

The separation of compounds was achieved with triethyl ammonium acetate (100 mM) buffer and acetonitrile with triethyl ammonium acetate (10 mM) gradient elution. B was held at 95% for 5 min, and then was eluted from 95% to 20% in 12 min.

5.2. HPLC chromatograms

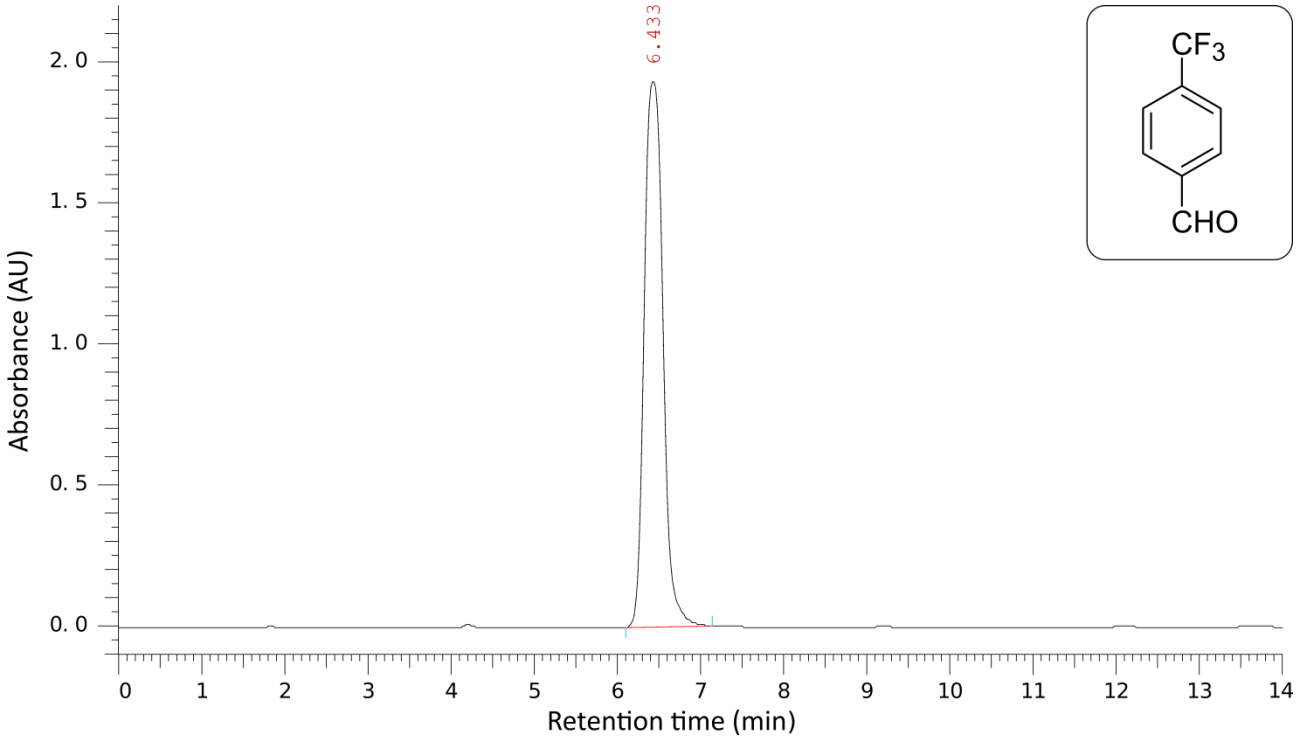


Fig. S77 Chromatogram of 4-(trifluoromethyl)benzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 1.

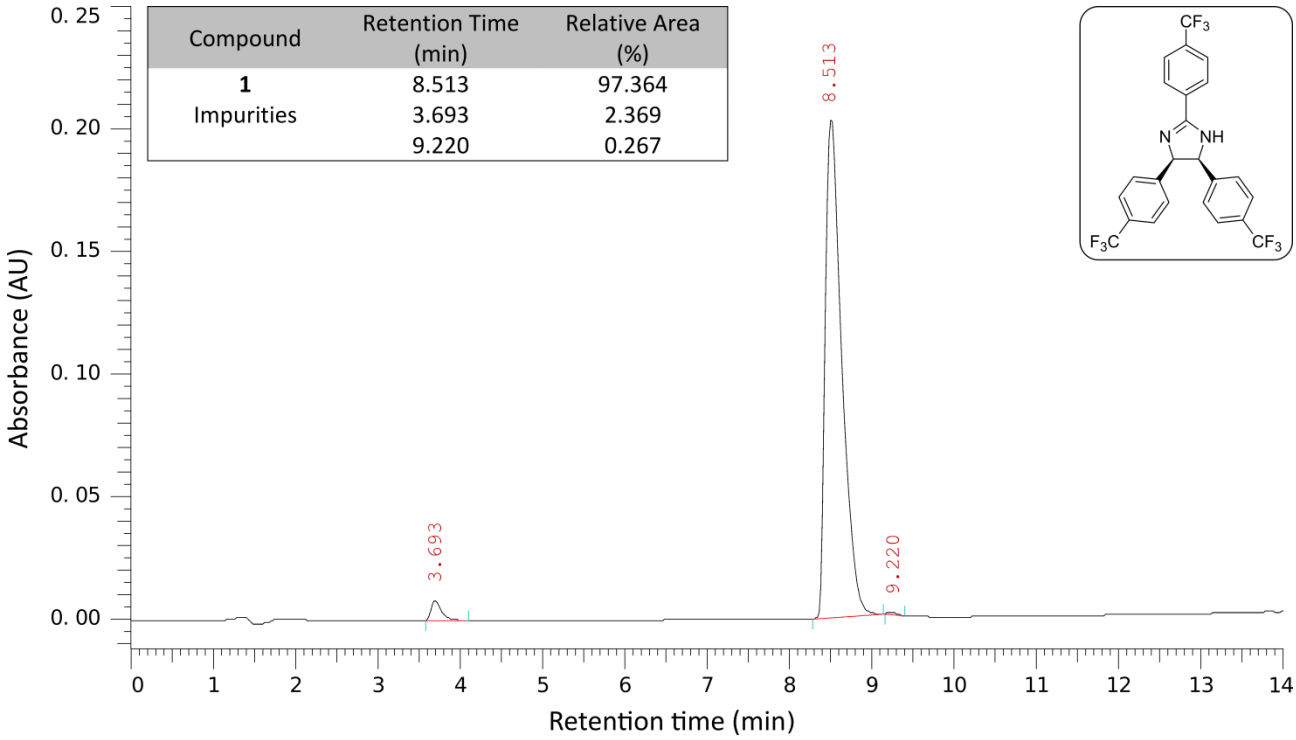


Fig. S78 Chromatogram of **1** after recrystallisation at 250 nm with the table of peaks and structure in insert. The compound was monitored with Method 1.

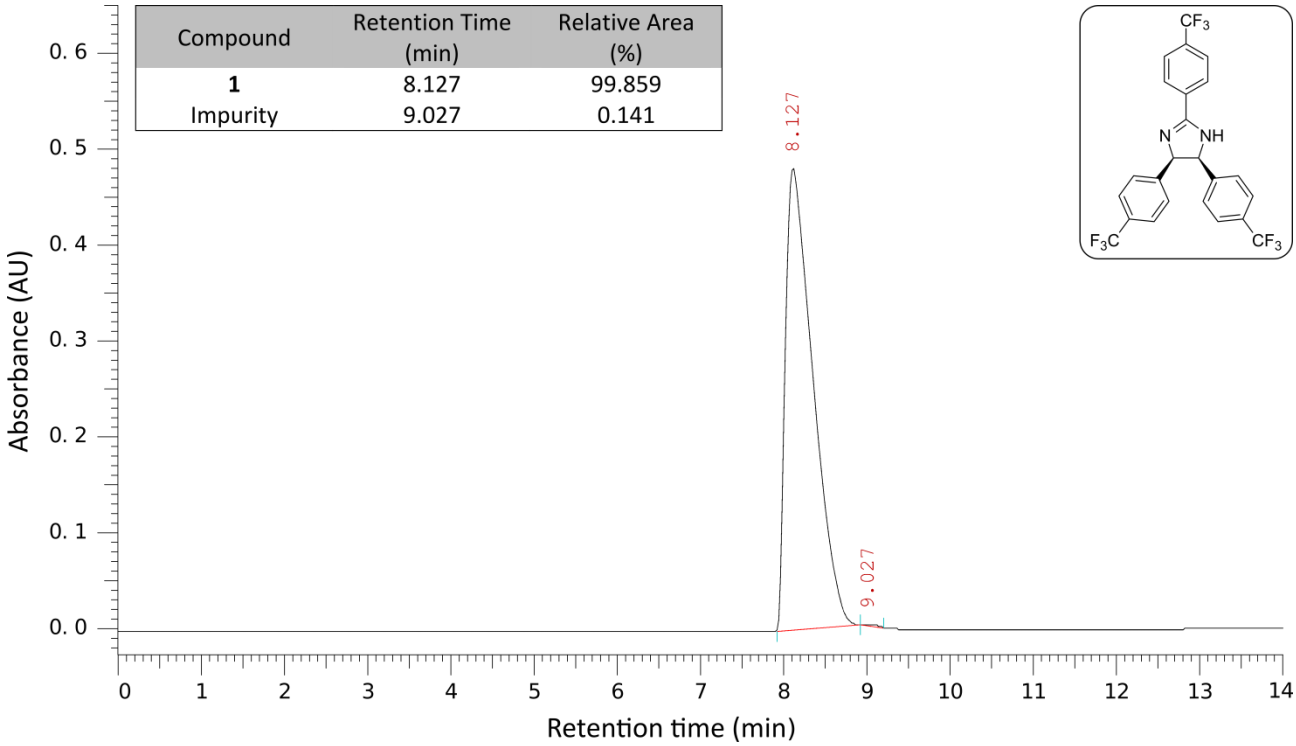


Fig. S79 Chromatogram of **1** after preparative HPLC purification at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

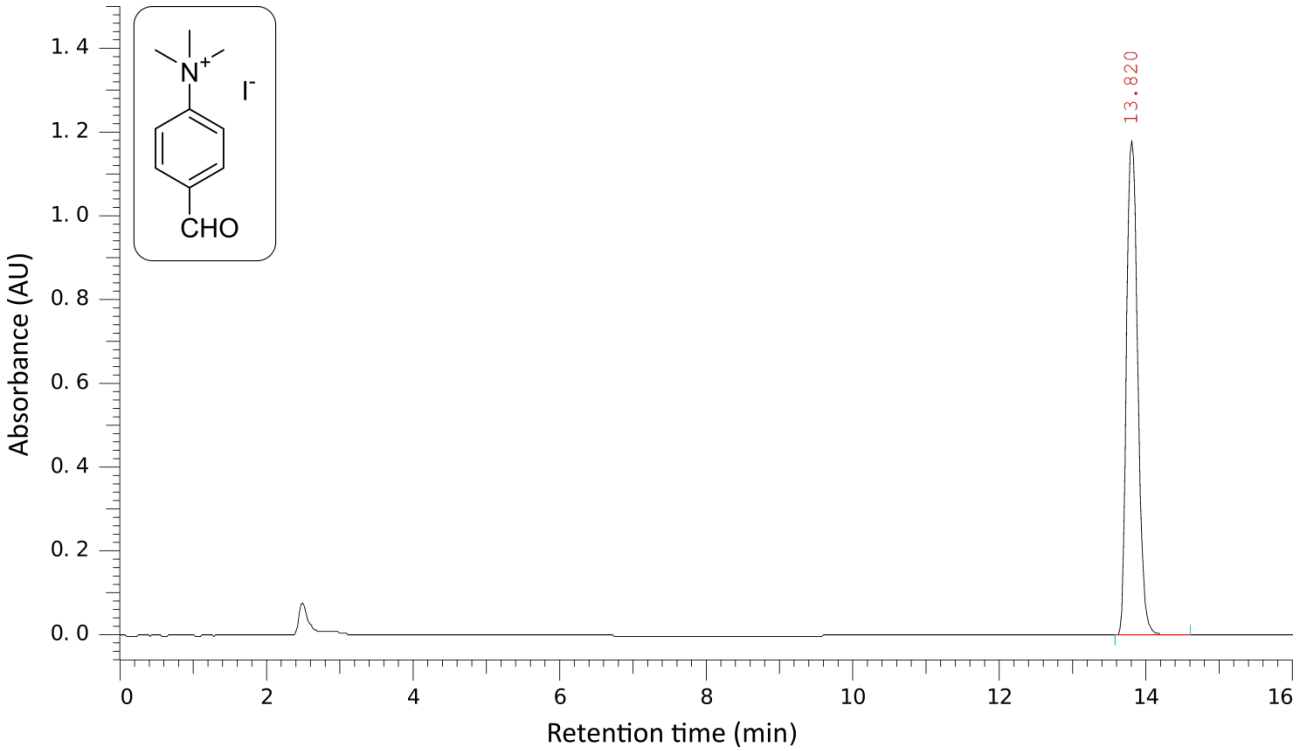
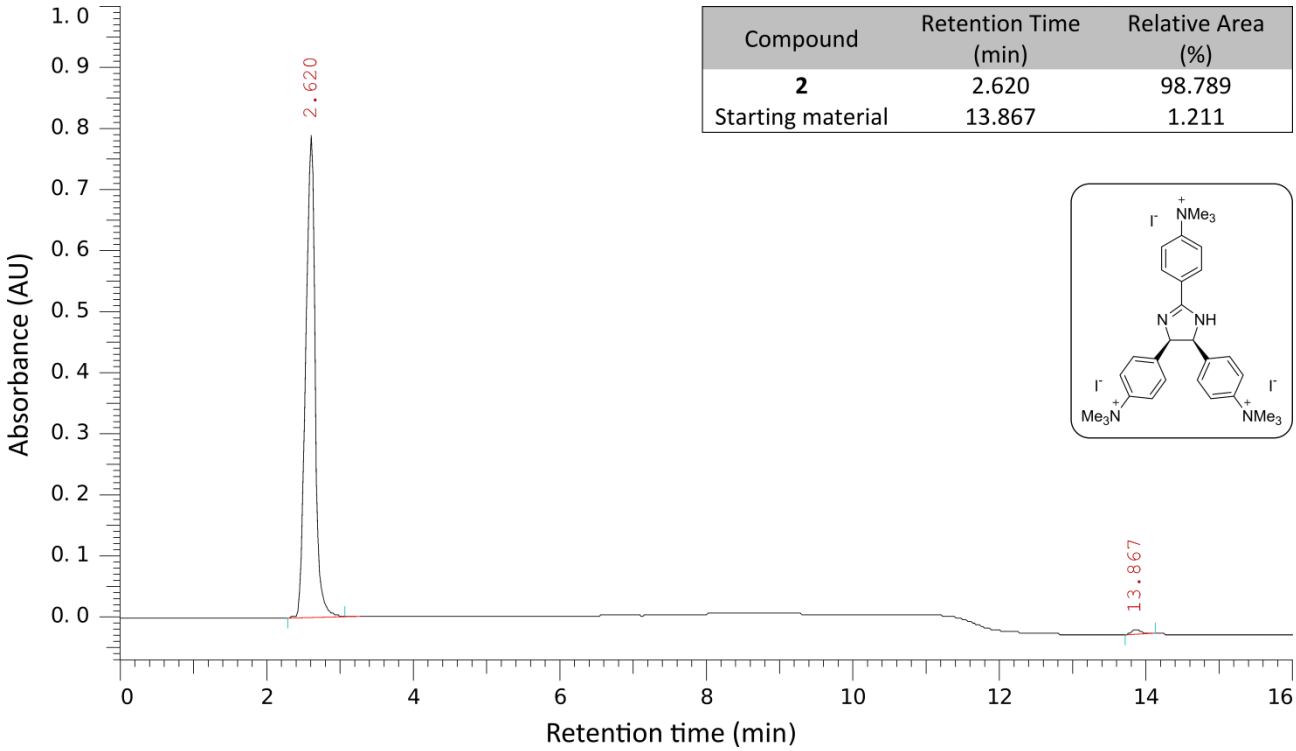


Fig. S80 Chromatogram of 4-formyl-*N*,*N*,*N*-trimethylanilinium iodide at 280 nm with the structure in insert. The compound was monitored with Method 5.



Compound	Retention Time (min)	Relative Area (%)
2	2.620	98.789
Starting material	13.867	1.211

Fig. S81 Chromatogram of **2** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 5.

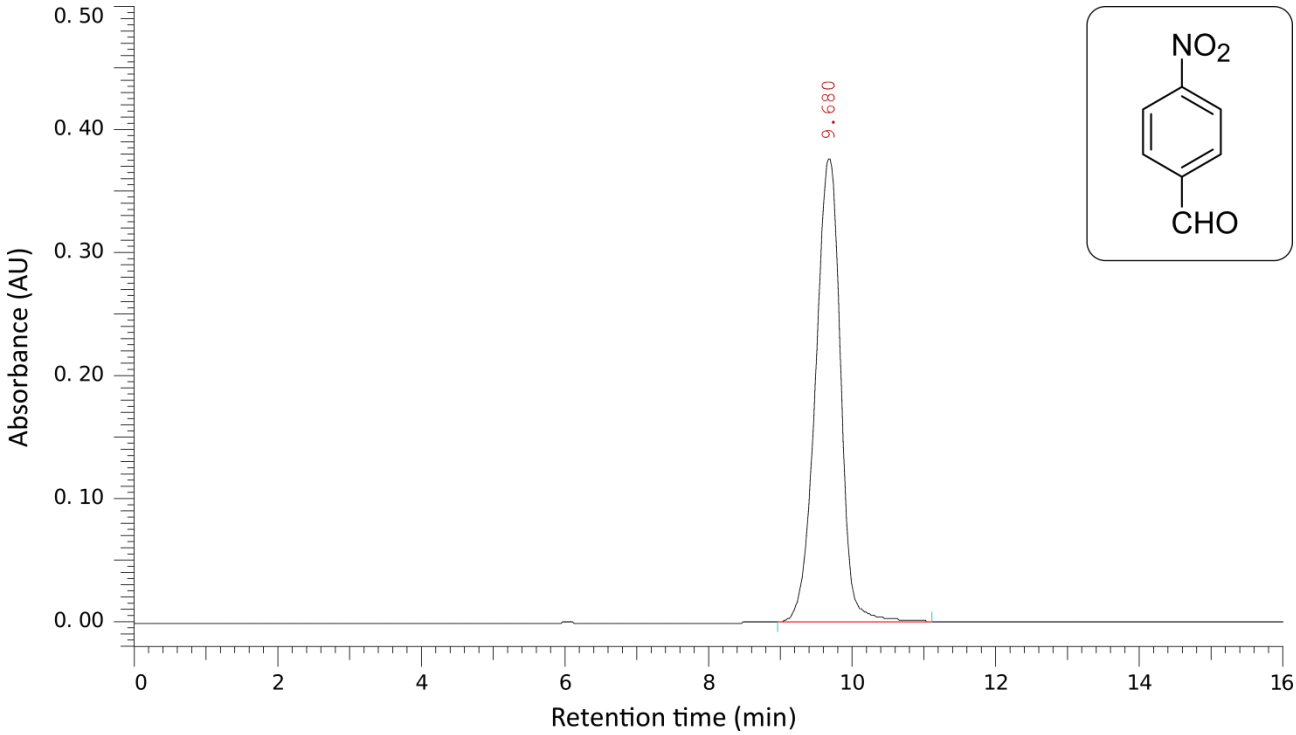


Fig. S82 Chromatogram of 4-nitrobenzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 2.

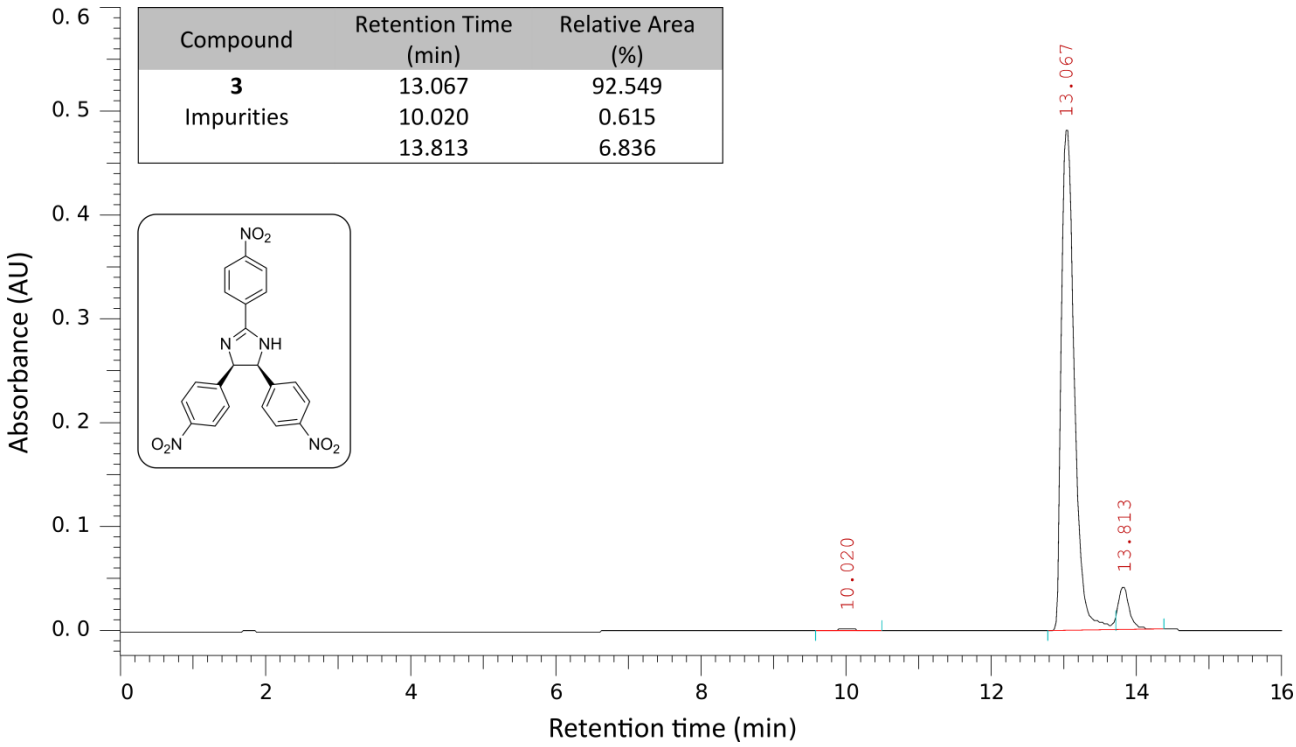


Fig. S83 Chromatogram of **3** after filtering the precipitated product at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 2.

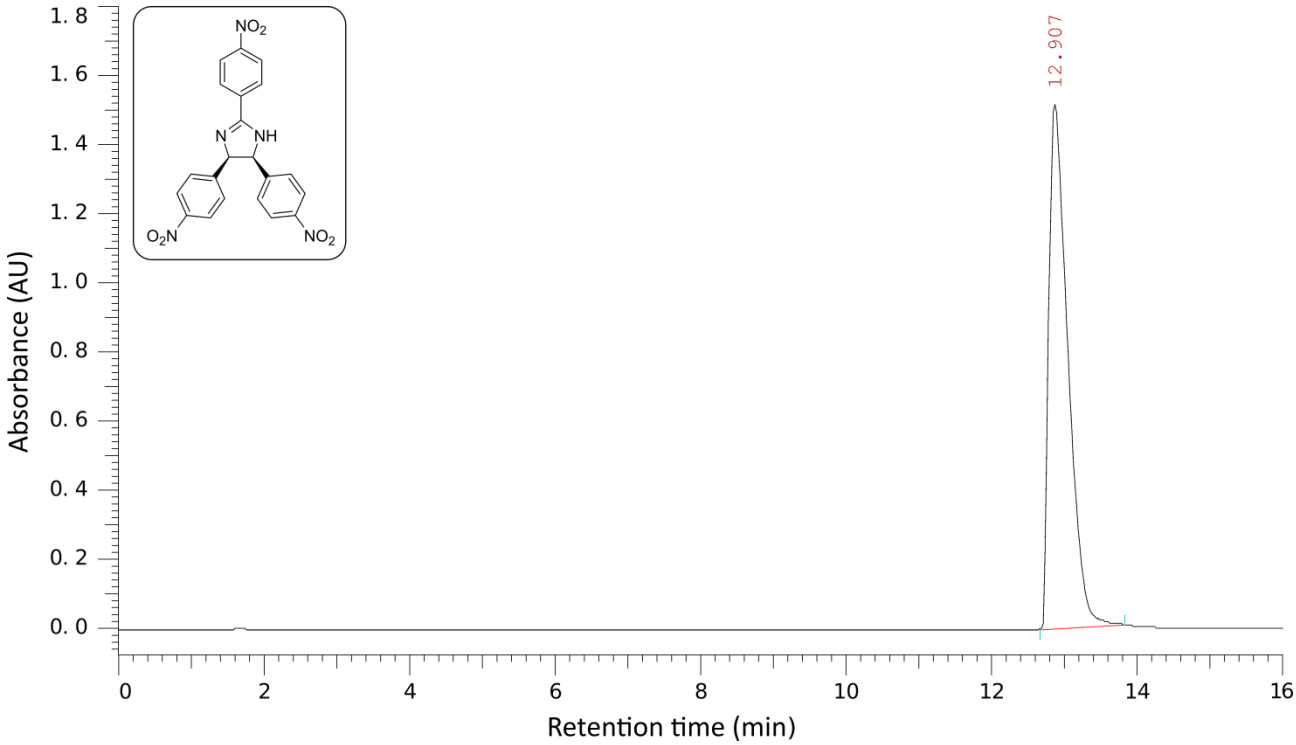


Fig. S84 Chromatogram of **3** after preparative HPLC purification at 250 nm with the structure in insert. The compound was monitored with Method 2.

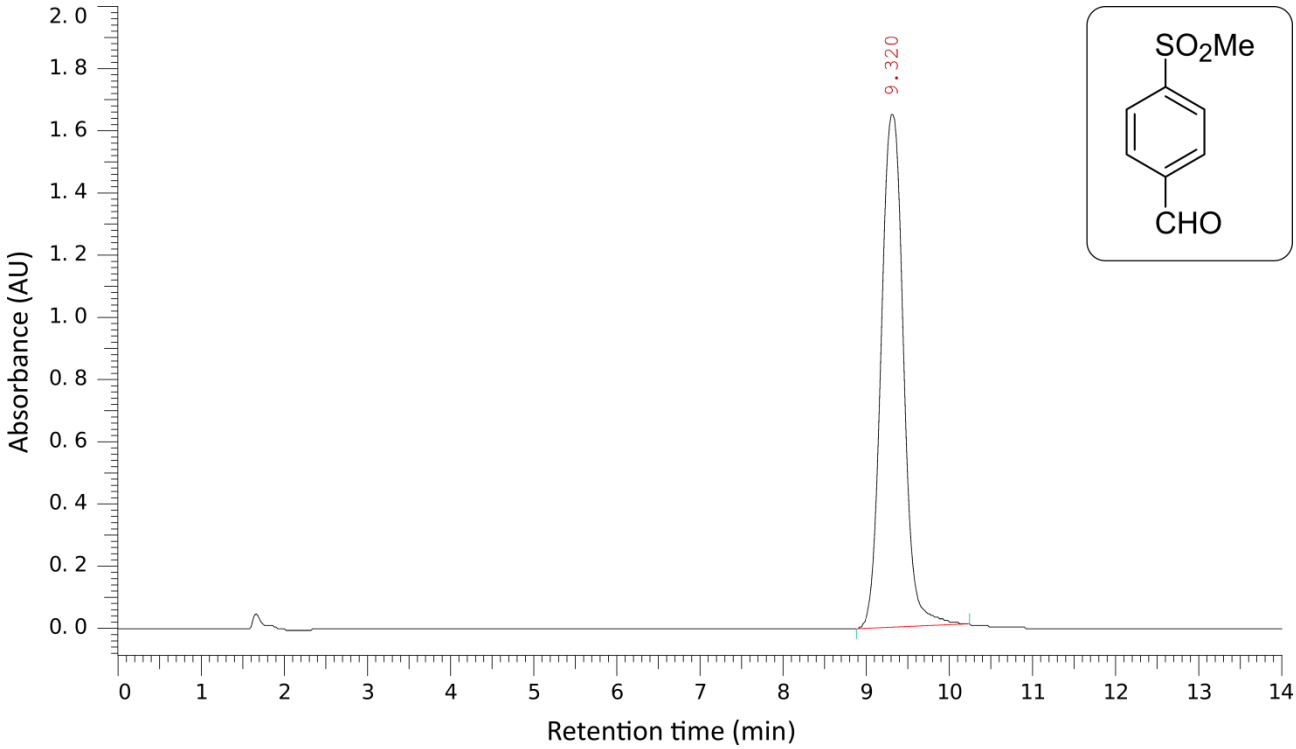


Fig. S85 Chromatogram of 4-(methylsulfonyl)benzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 3.

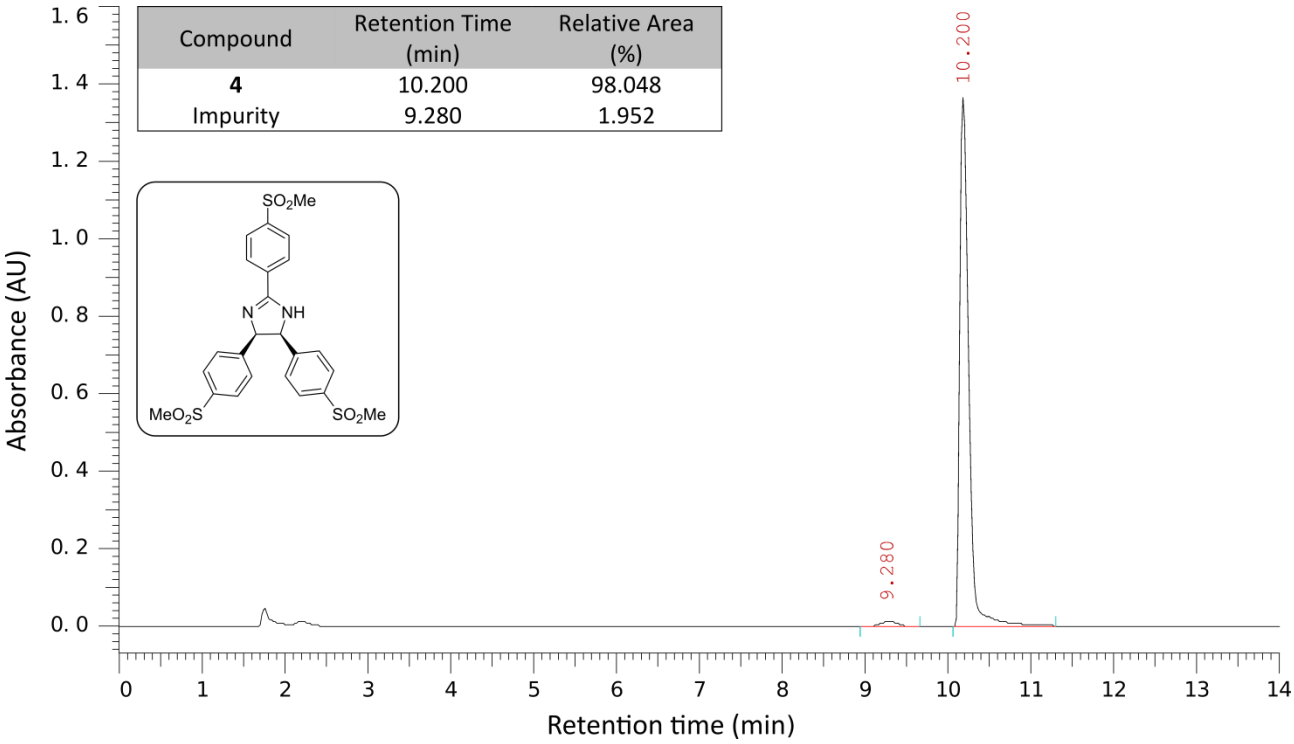


Fig. S86 Chromatogram of **4** after filtering the precipitated product at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 3.

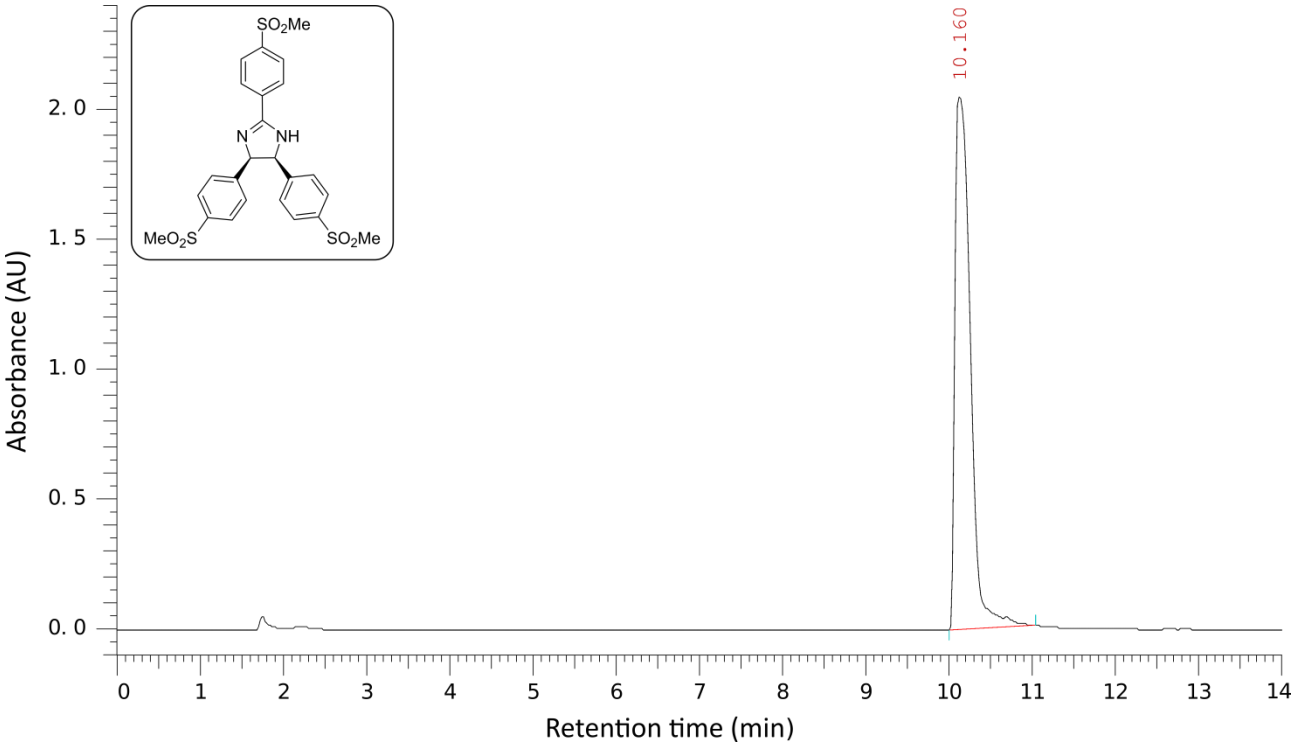


Fig. S87 Chromatogram of **4** after preparative HPLC purification at 250 nm with the structure in insert. The compound was monitored with Method 3.

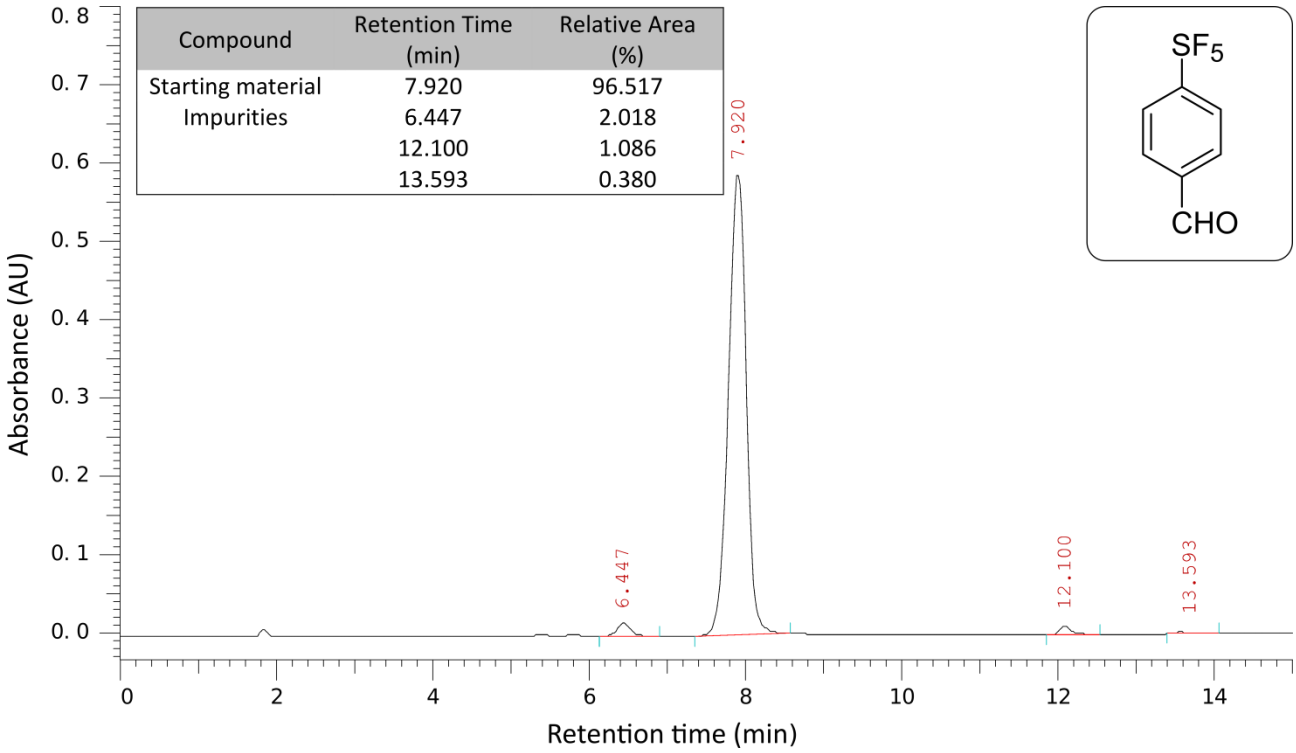


Fig. S88 Chromatogram of 4-(pentafluorosulfanyl)benzaldehyde at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

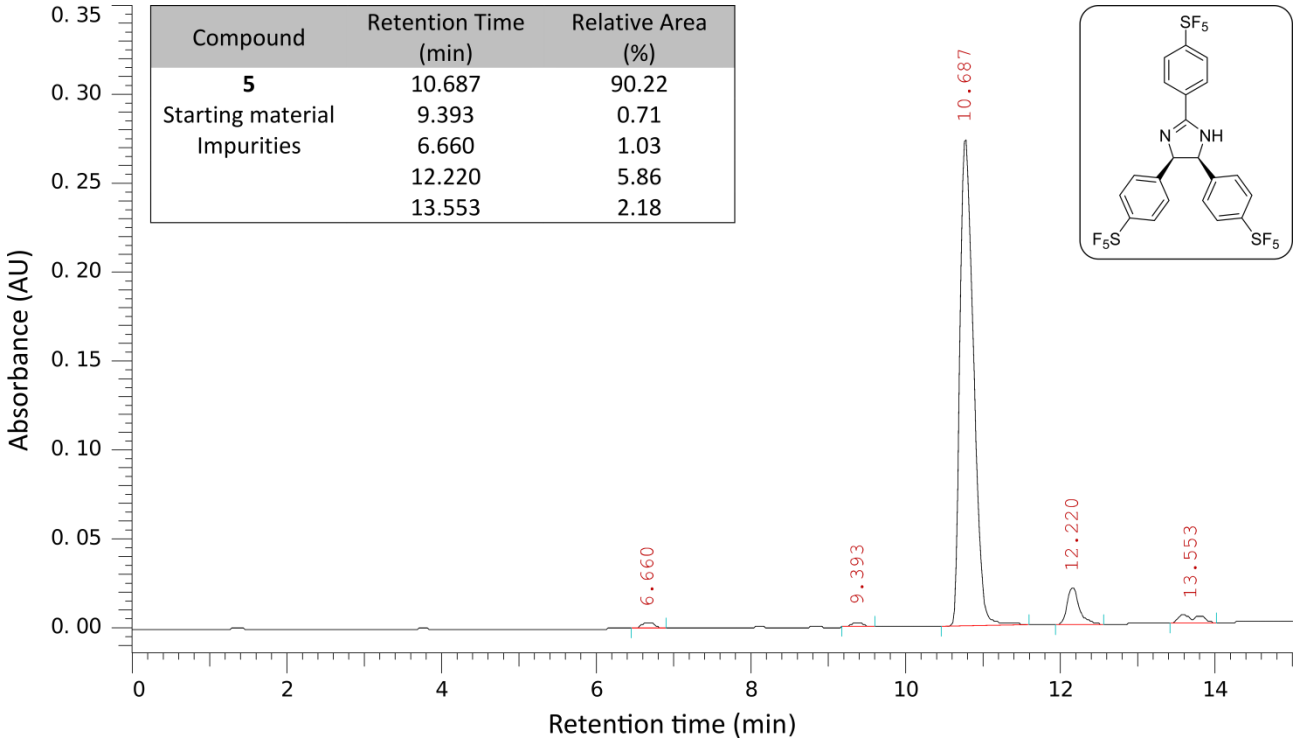


Fig. S89 Chromatogram of **5** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

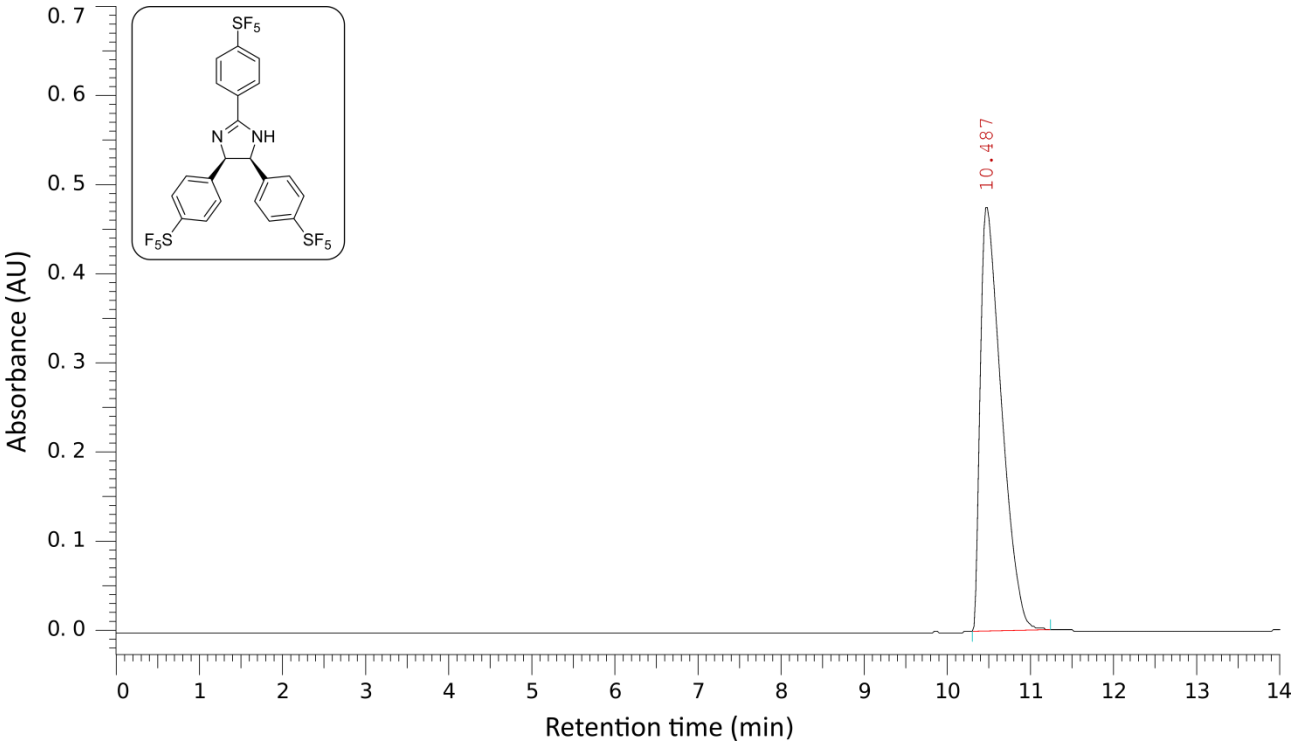


Fig. S90 Chromatogram of **5** after preparative HPLC purification at 250 nm with the structure in insert. The compound was monitored with Method 1.

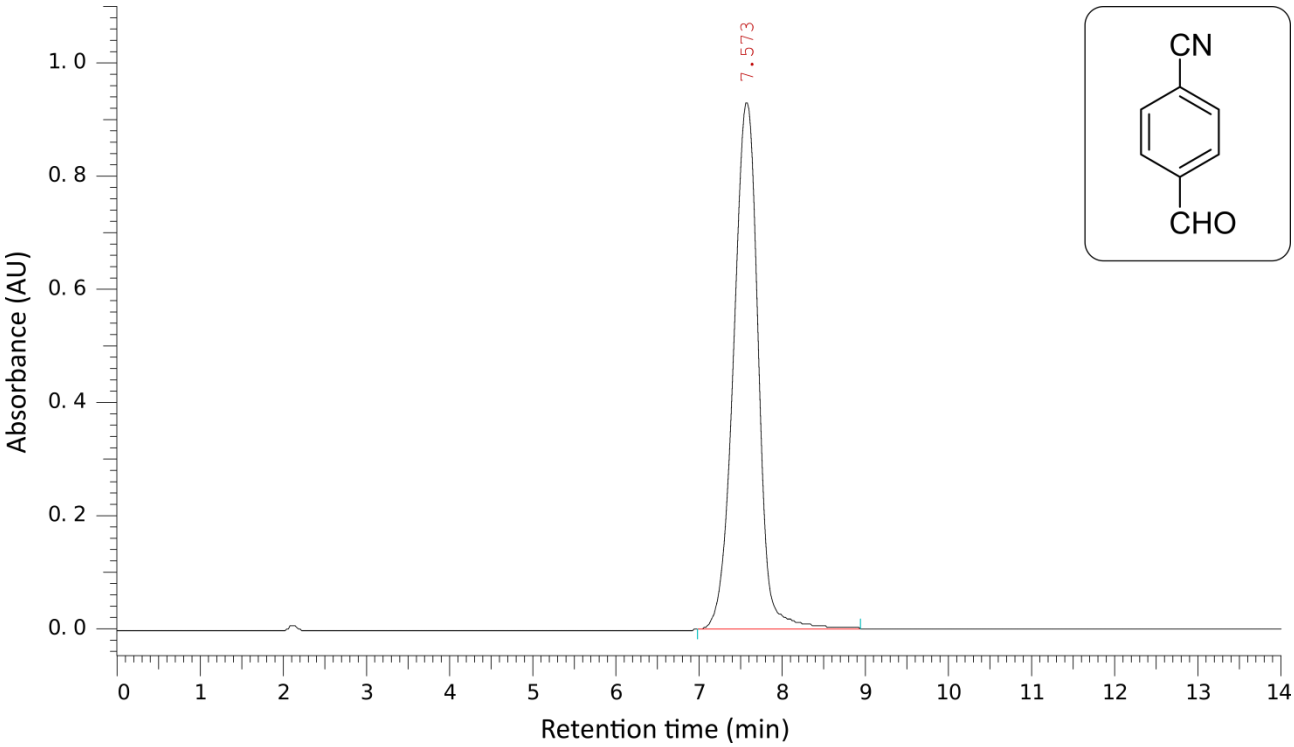


Fig. S91 Chromatogram of 4-cyanobenzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 2.

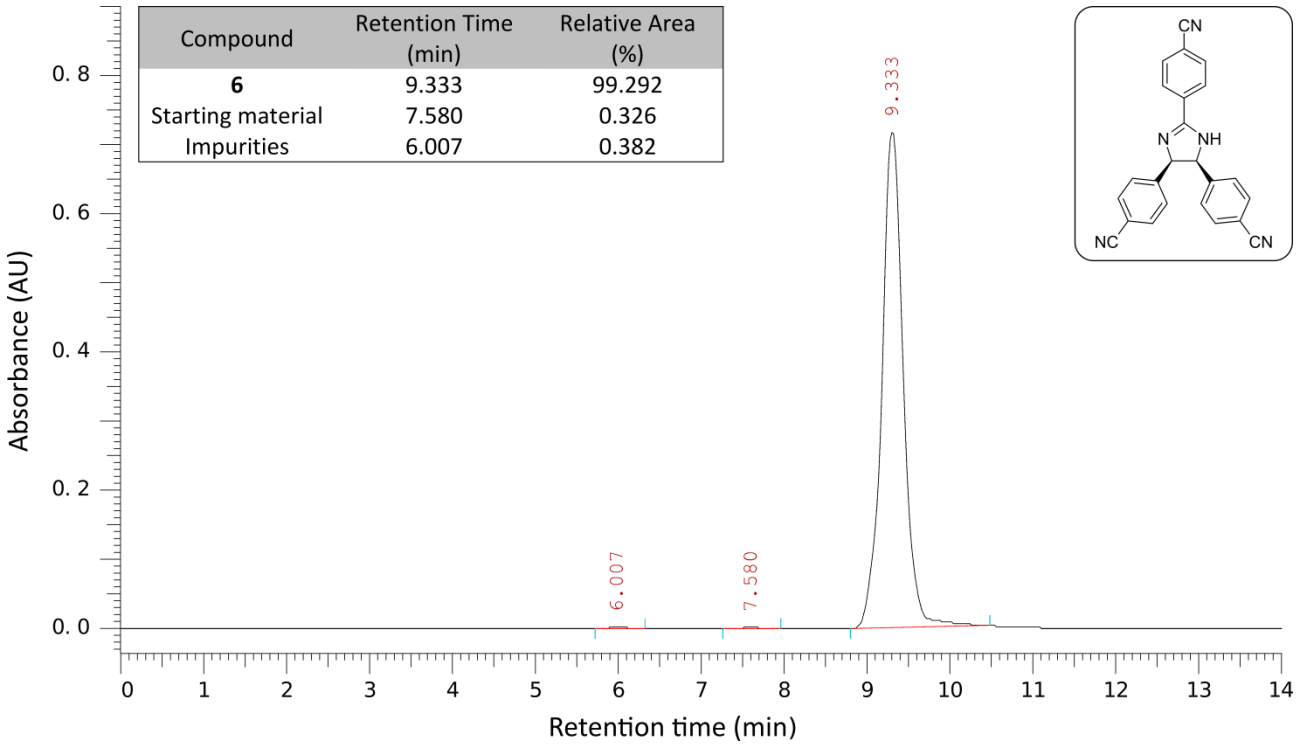


Fig. S92 Chromatogram of **6** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 2.

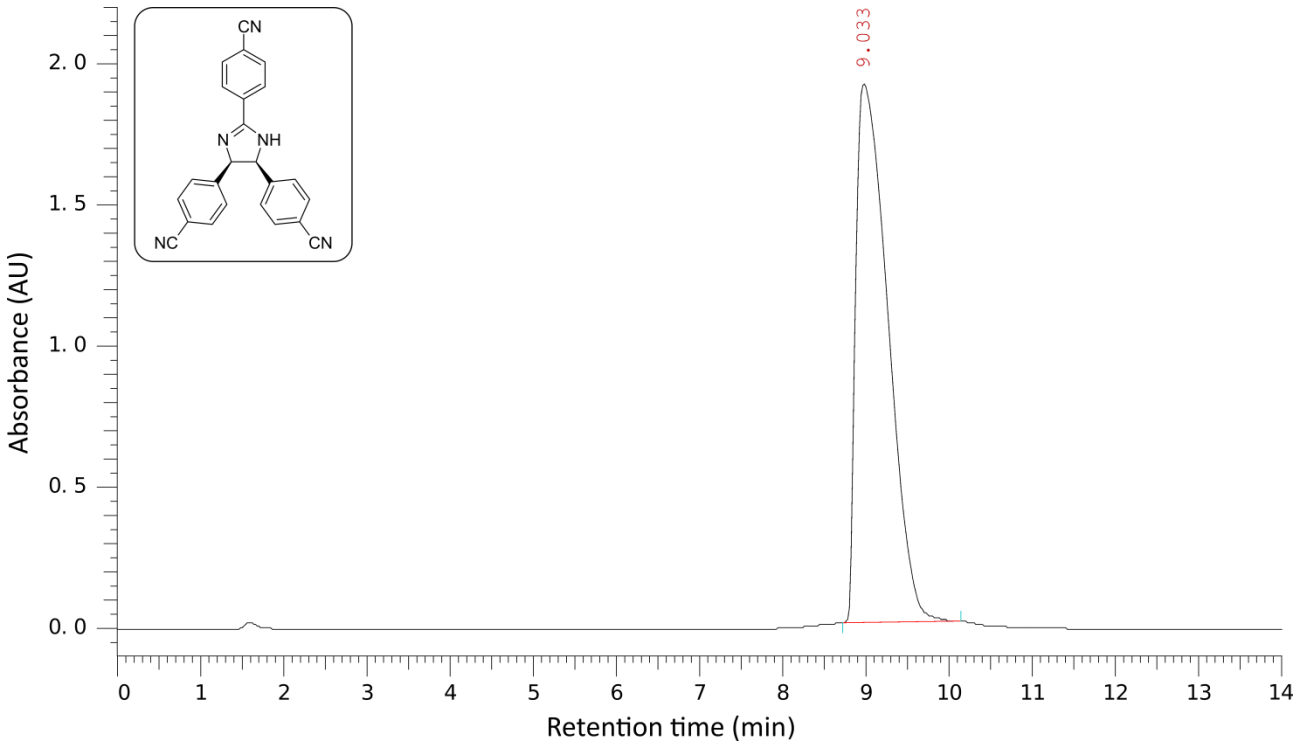


Fig. S93 Chromatogram of **6** after preparative HPLC purification at 250 nm with the structure in insert. The compound was monitored with Method 2.

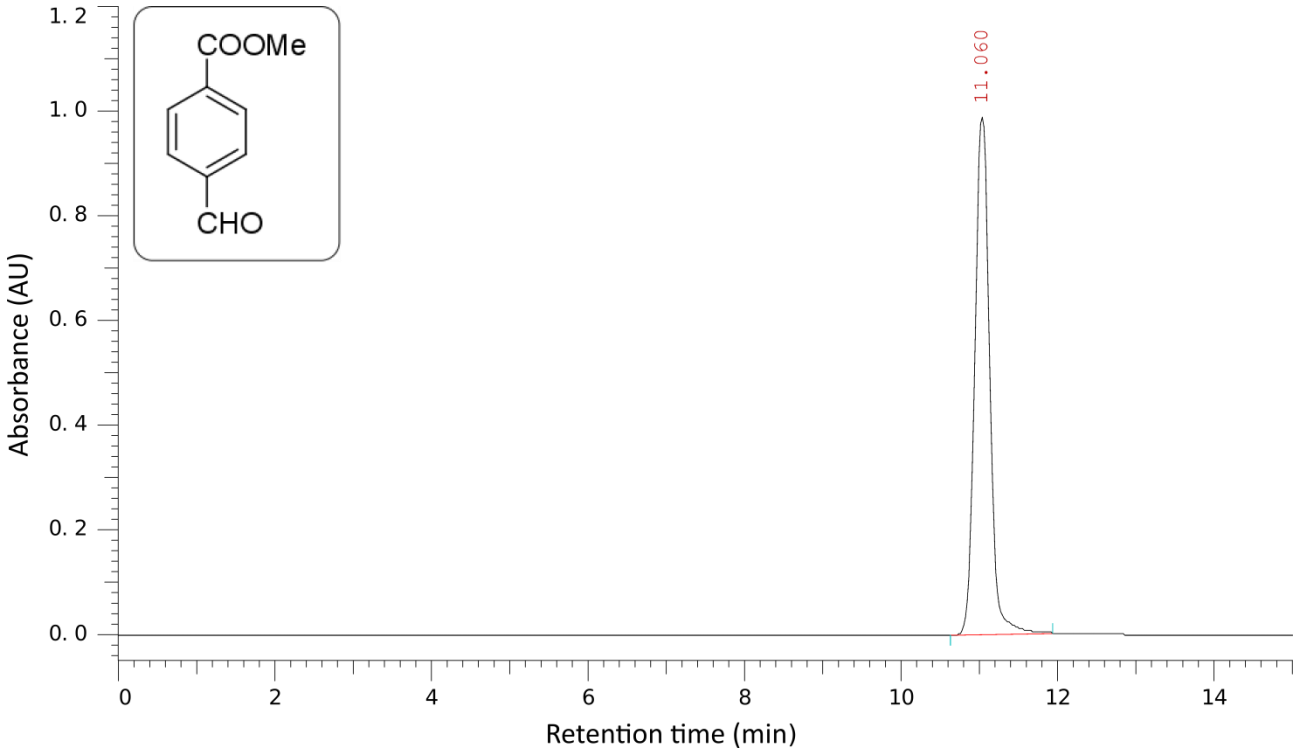


Fig. S94 Chromatogram of 4-formylbenzoate at 250 nm with the structure in insert. The compound was monitored with Method 2.

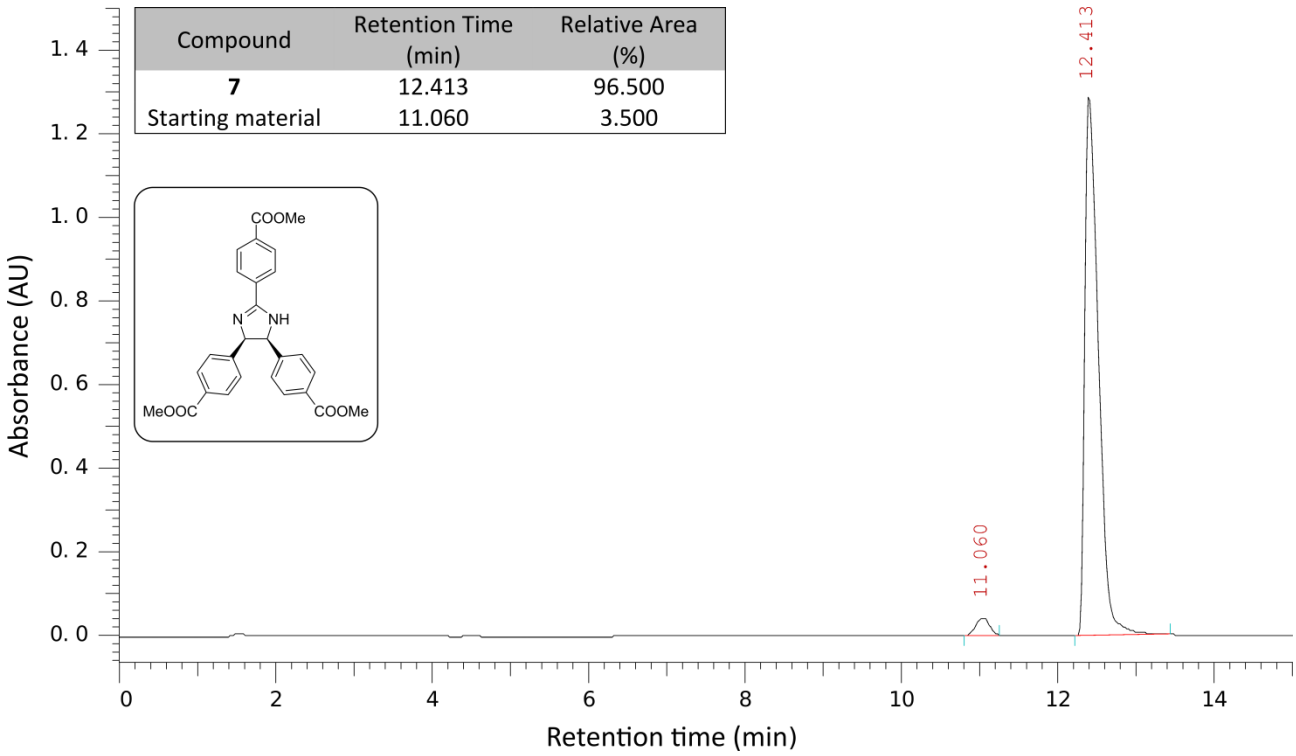


Fig. S95 Chromatogram of **7** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 2.

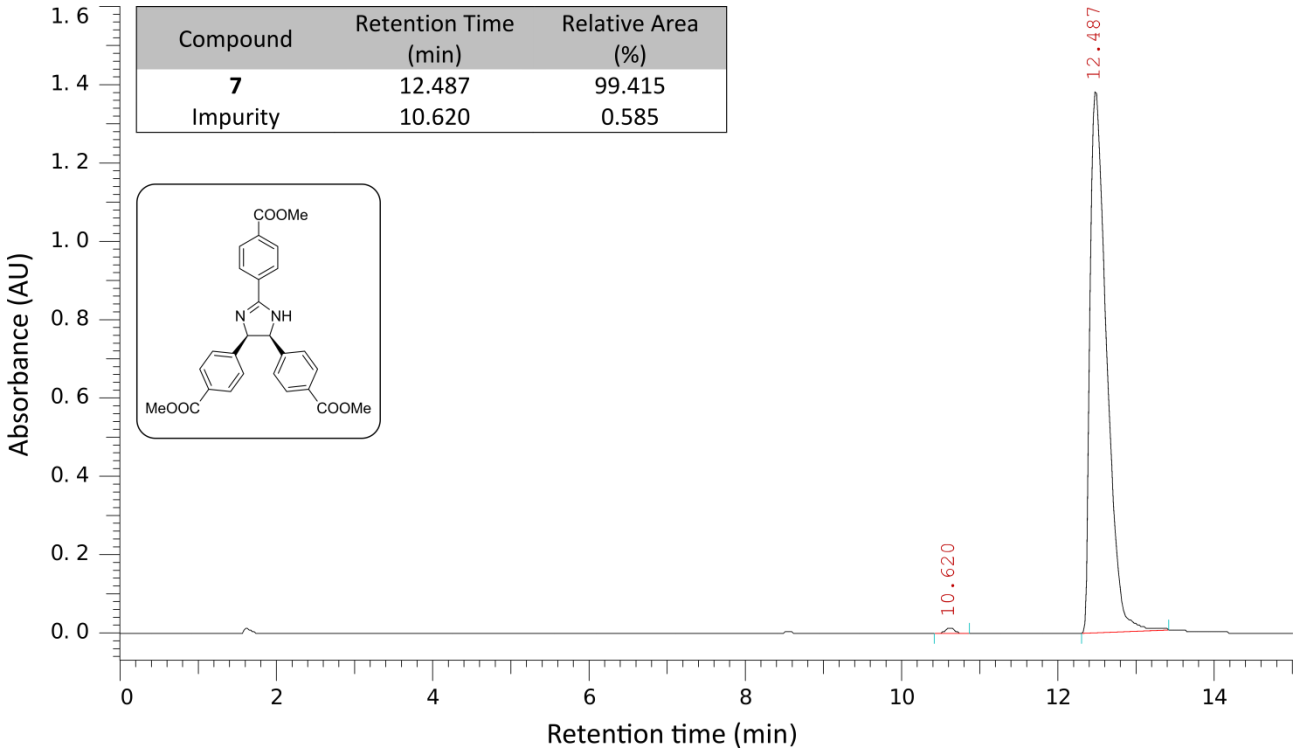


Fig. S96 Chromatogram of **7** after preparative HPLC purification at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 2.

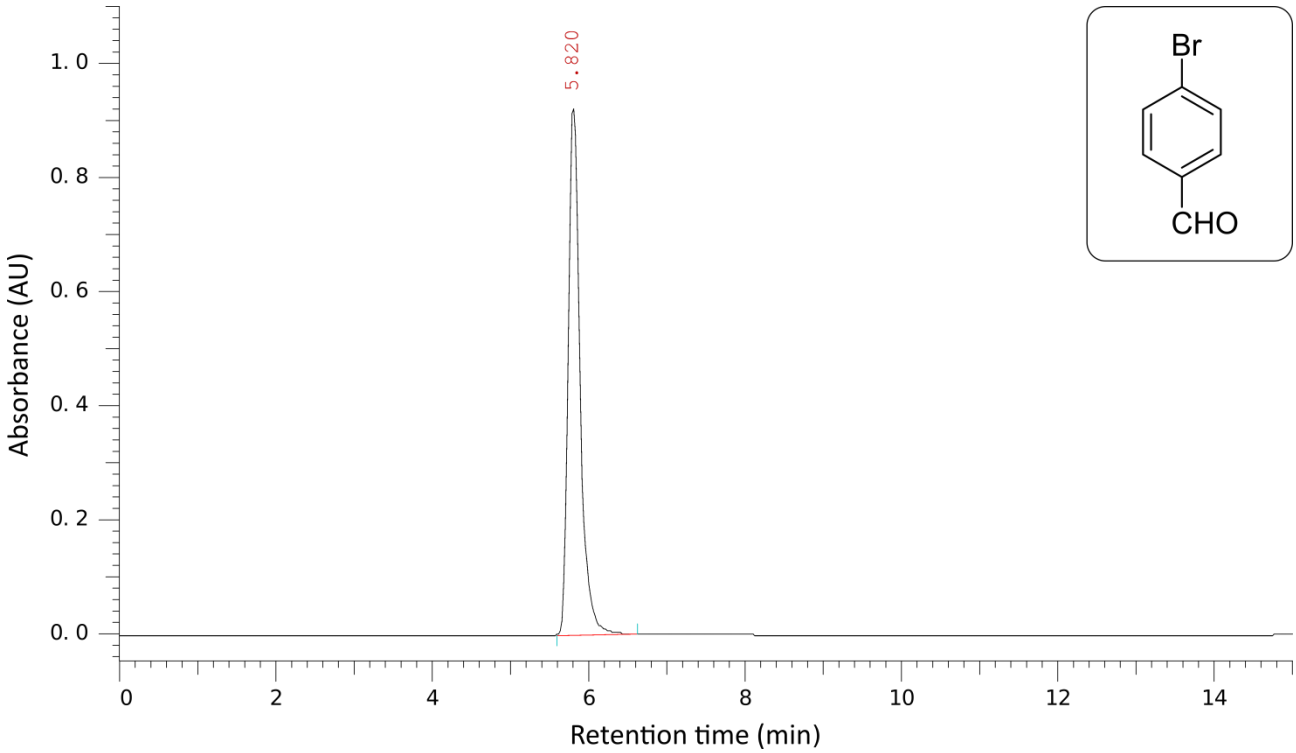


Fig. S97 Chromatogram of 4-bromobenzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 1.

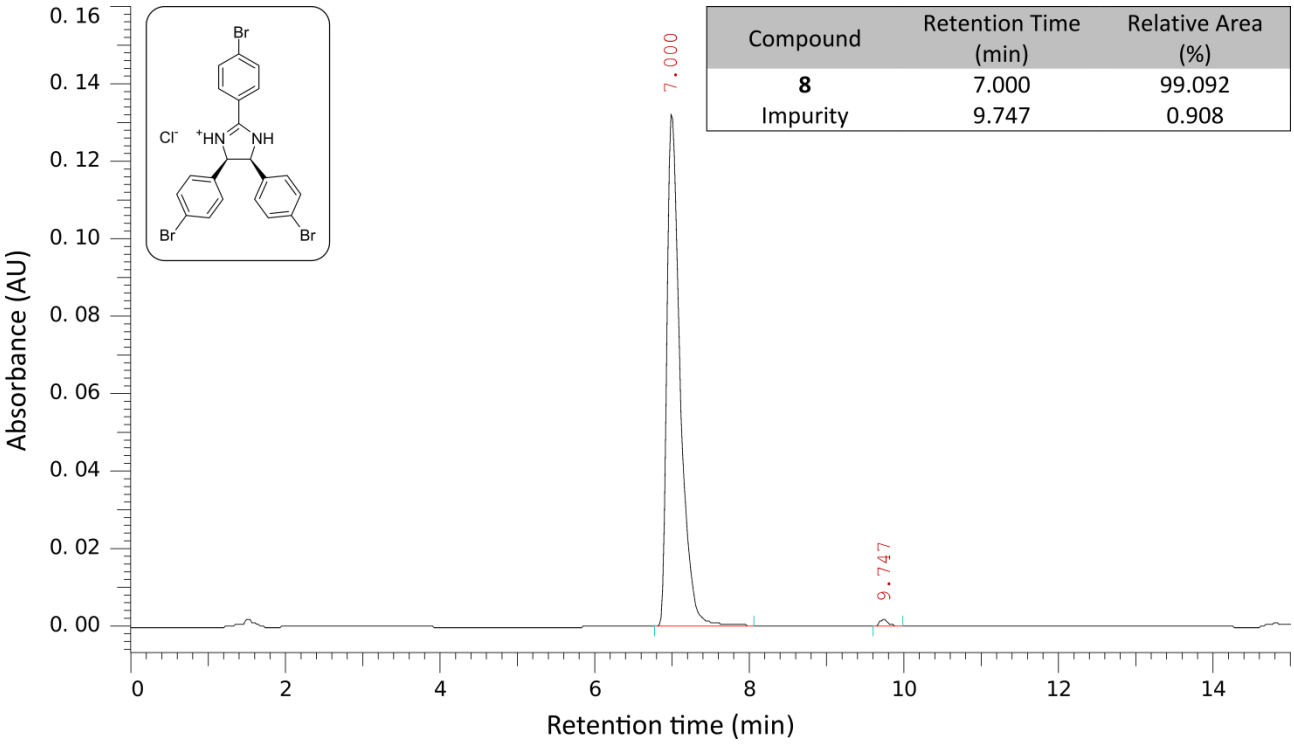


Fig. S98 Chromatogram of **8** at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

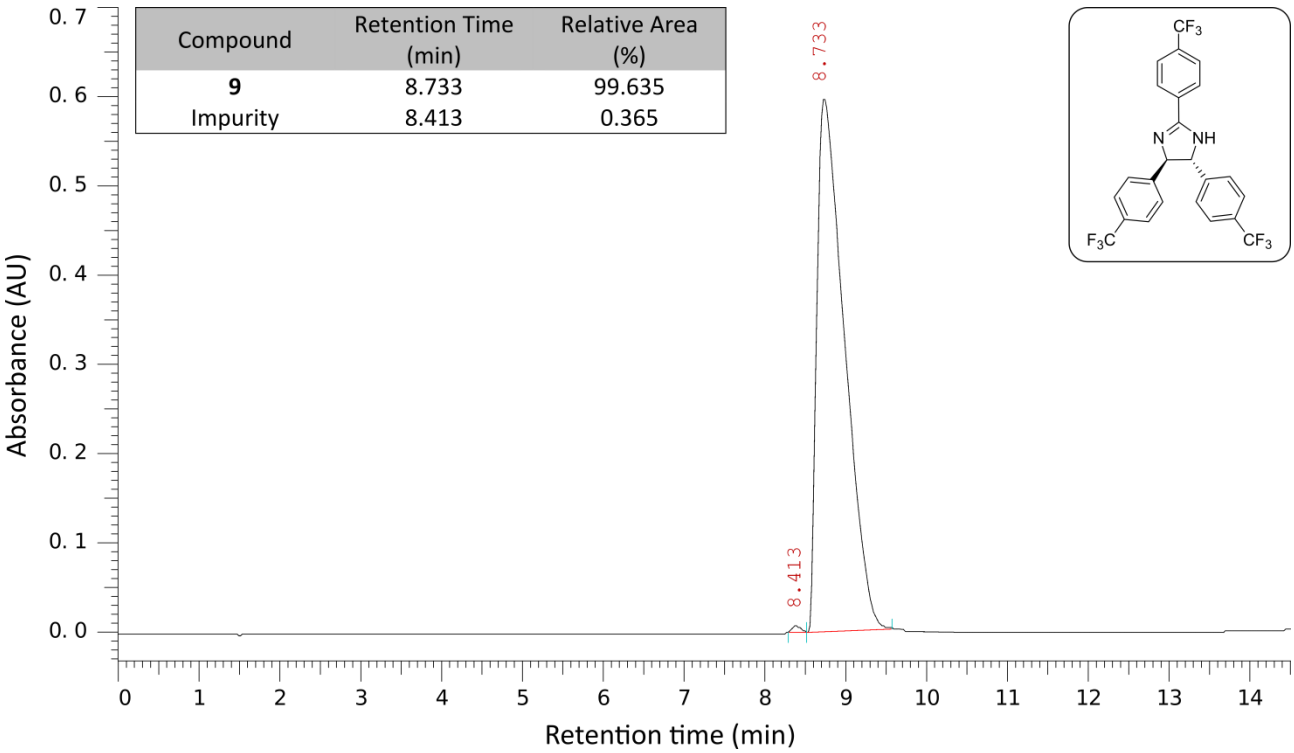


Fig. S99 Chromatogram of **9** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

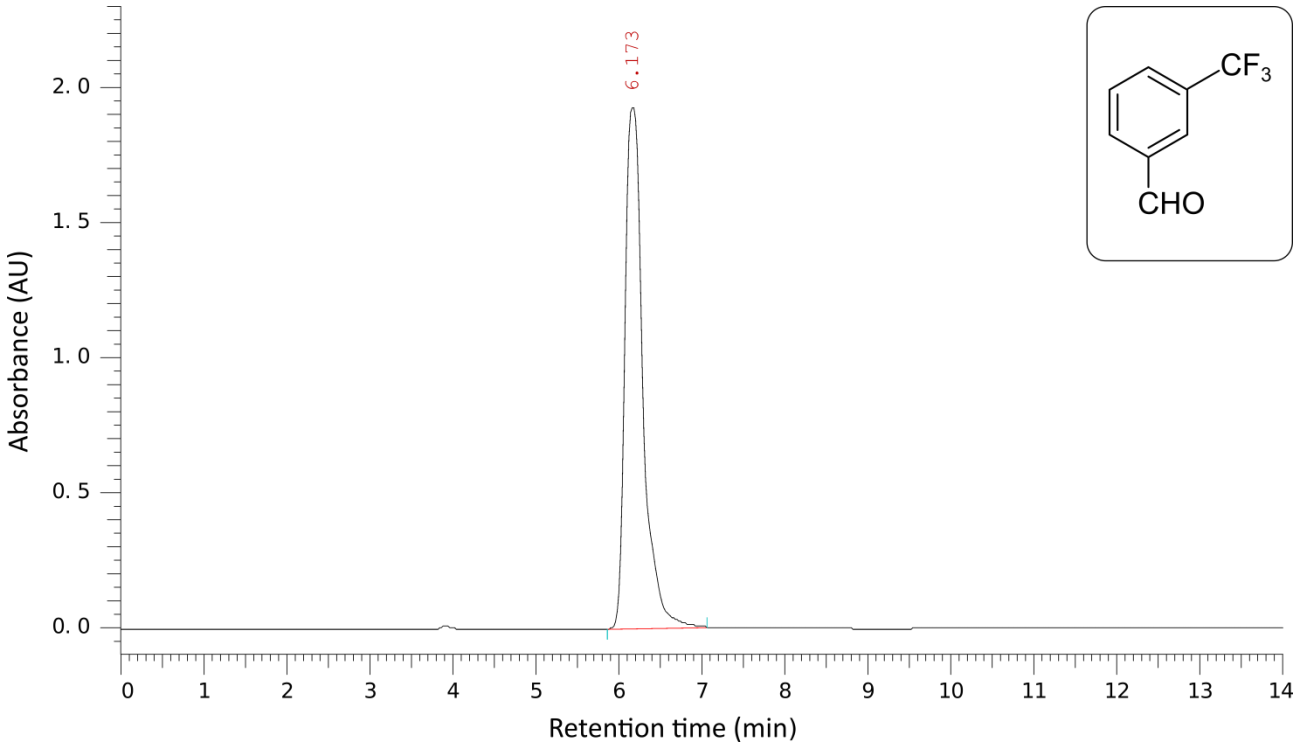


Fig. S100 Chromatogram of 3-(trifluoromethyl)benzaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 1.

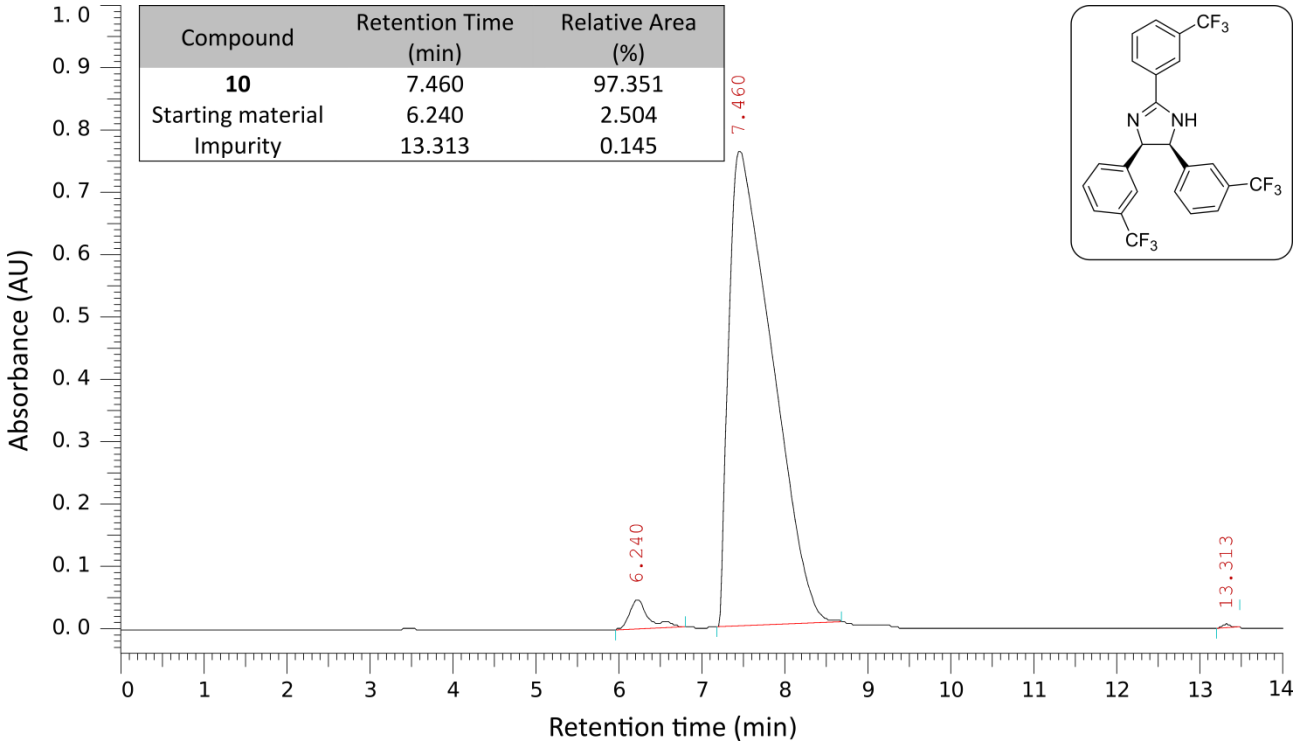


Fig. S101 Chromatogram of **10** at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

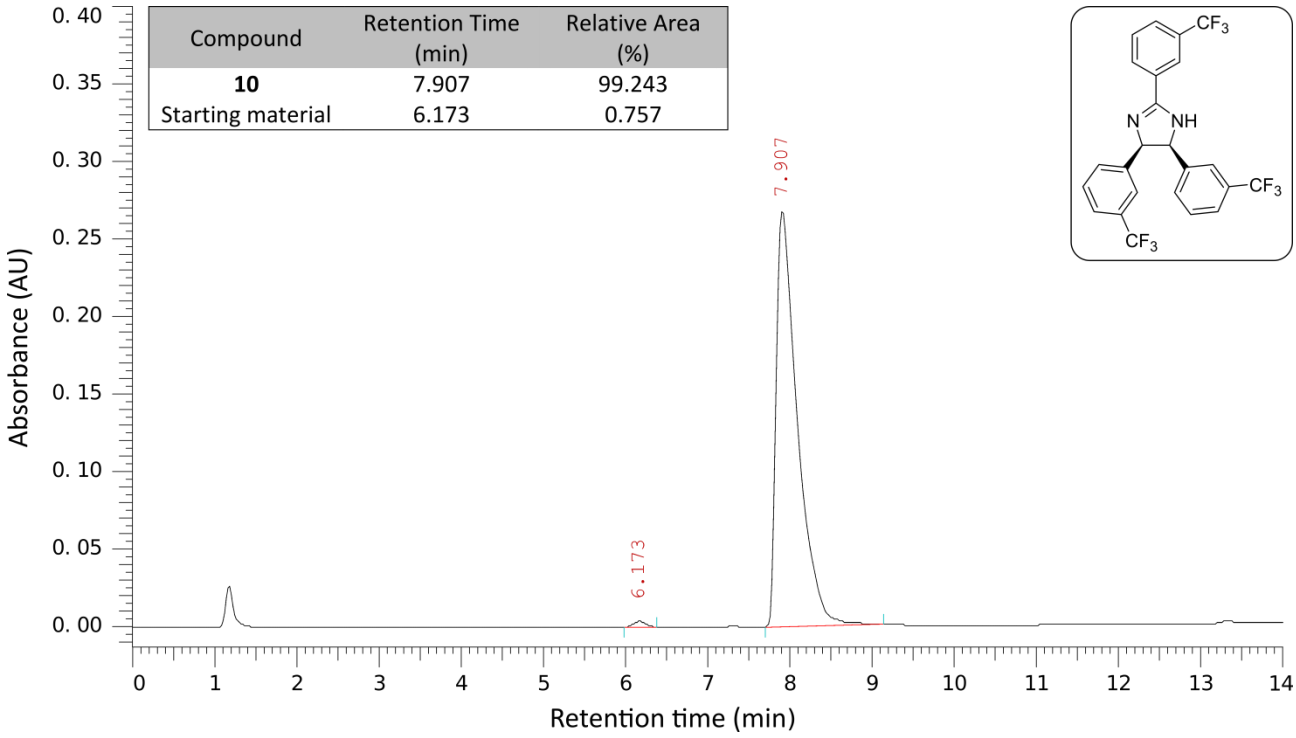


Fig. S102 Chromatogram of **10** after preparative HPLC purification at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

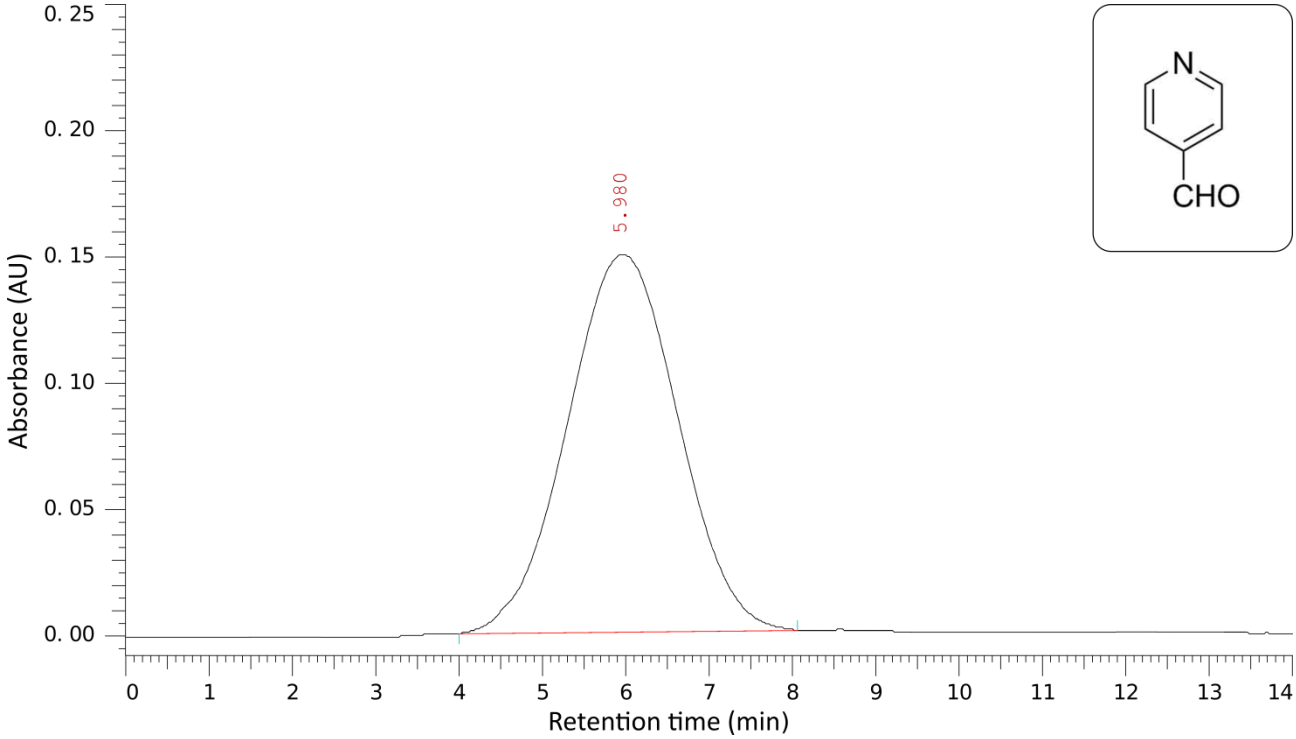


Fig. S103 Chromatogram of 4-formylpyridine at 250 nm with the structure in insert. The compound was monitored with Method 4.

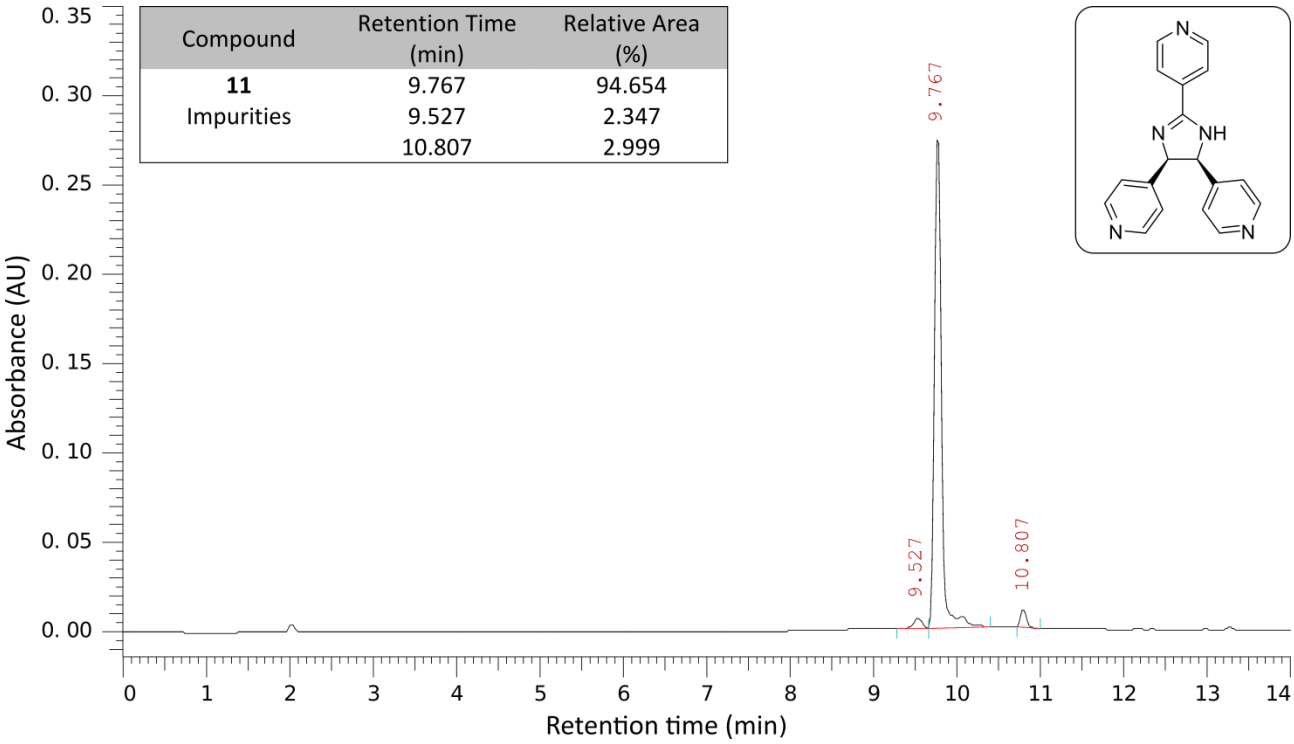


Fig. S104 Chromatogram of **11** after extraction at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 4.

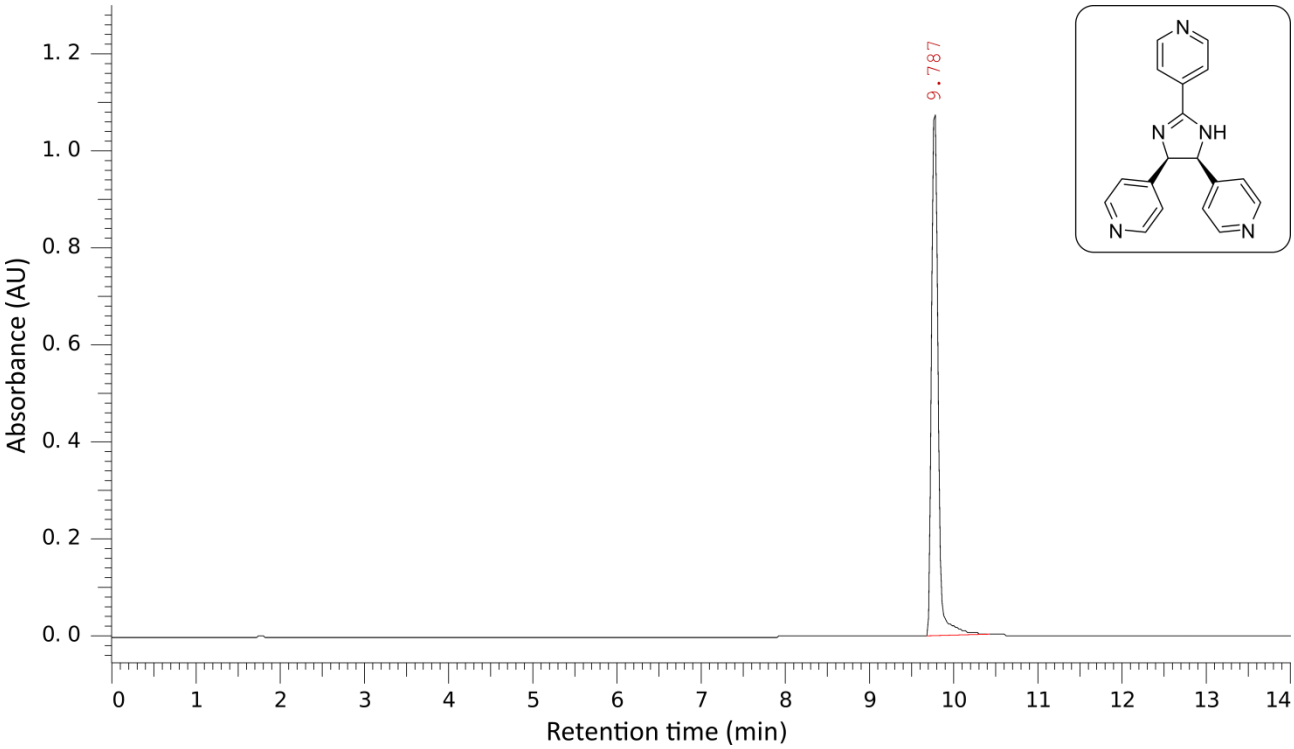


Fig. S105 Chromatogram of **11** after preparative HPLC purification at 250 nm with the structure in insert. The compound was monitored with Method 4.

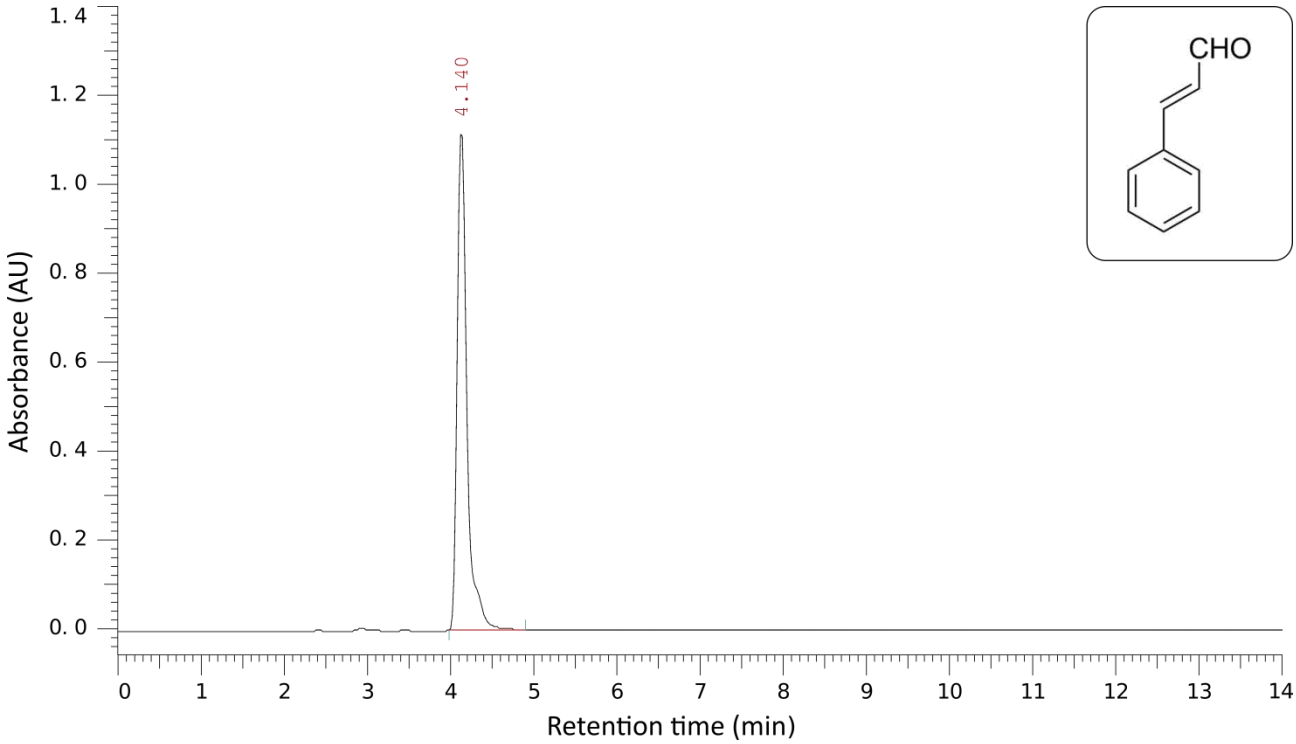


Fig. S106 Chromatogram of cinnamaldehyde at 250 nm with the structure in insert. The compound was monitored with Method 1.

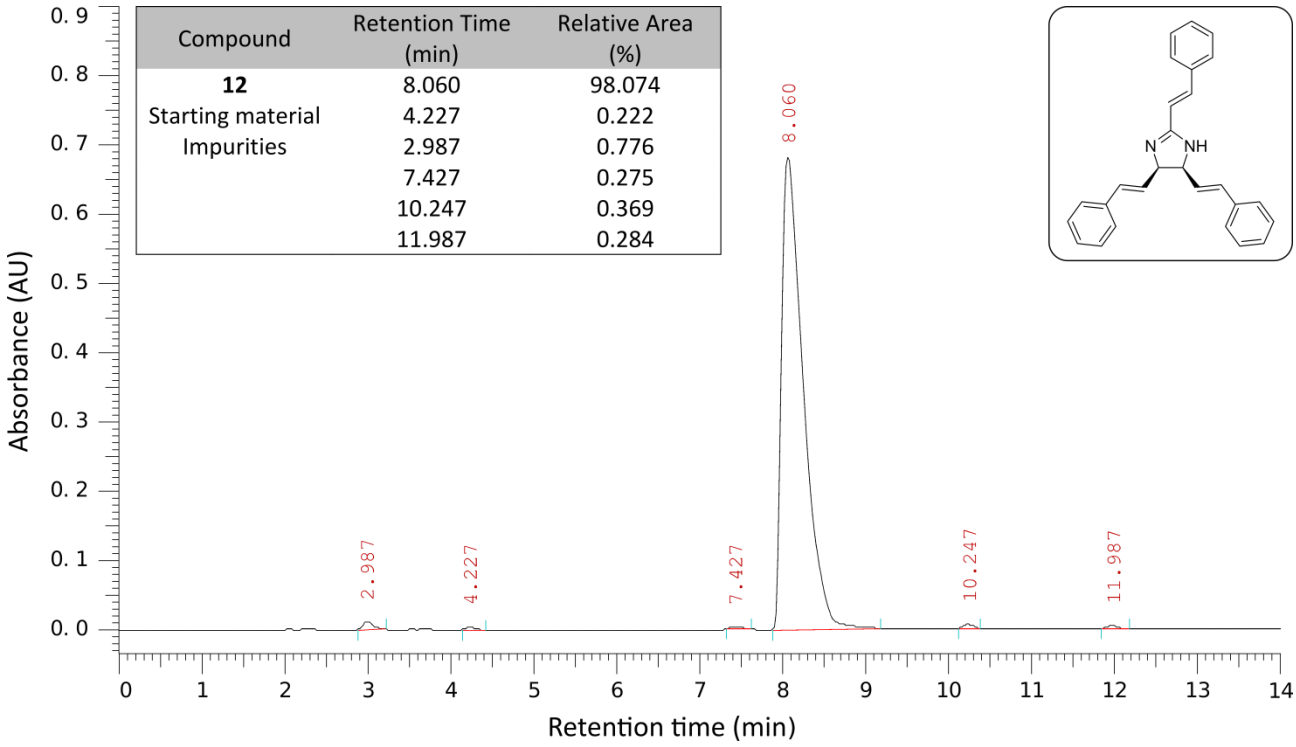


Fig. S107 Chromatogram of **12** after recrystallisation at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

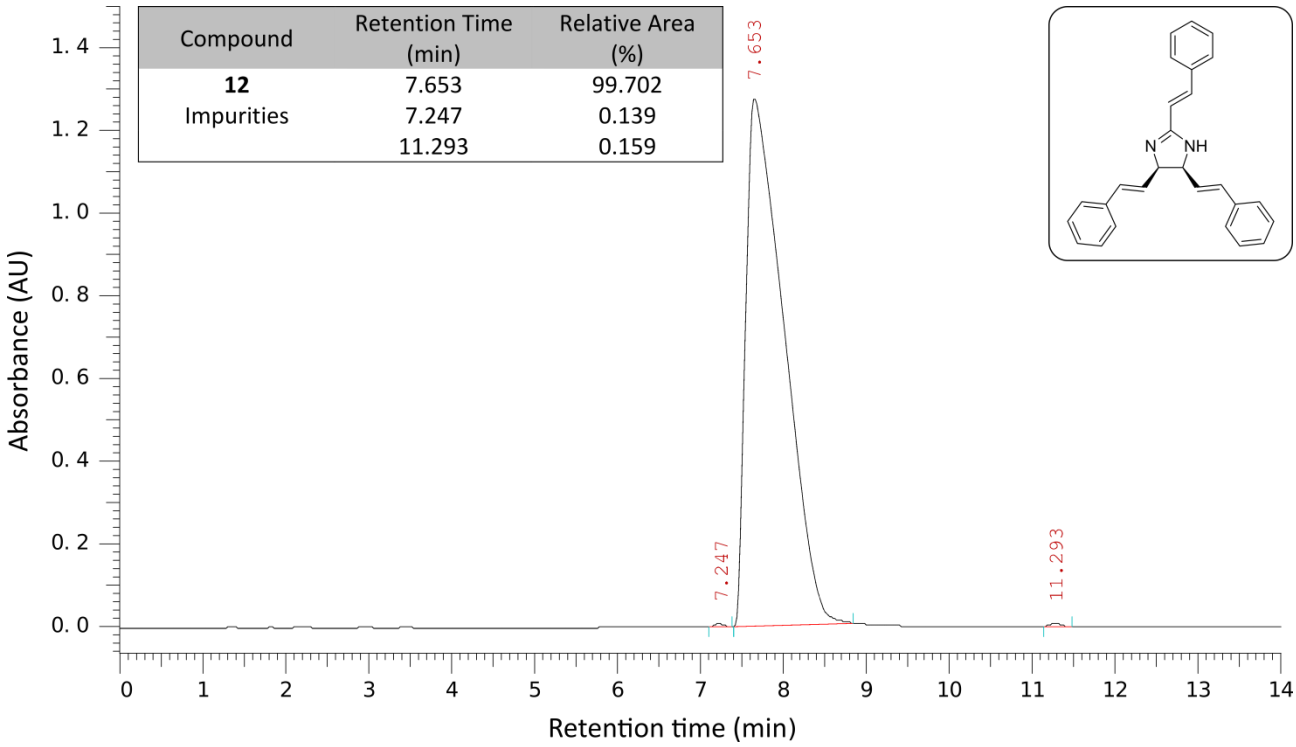


Fig. S108 Chromatogram of **12** after preparative HPLC purification at 250 nm with the table of peaks and the structure in insert. The compound was monitored with Method 1.

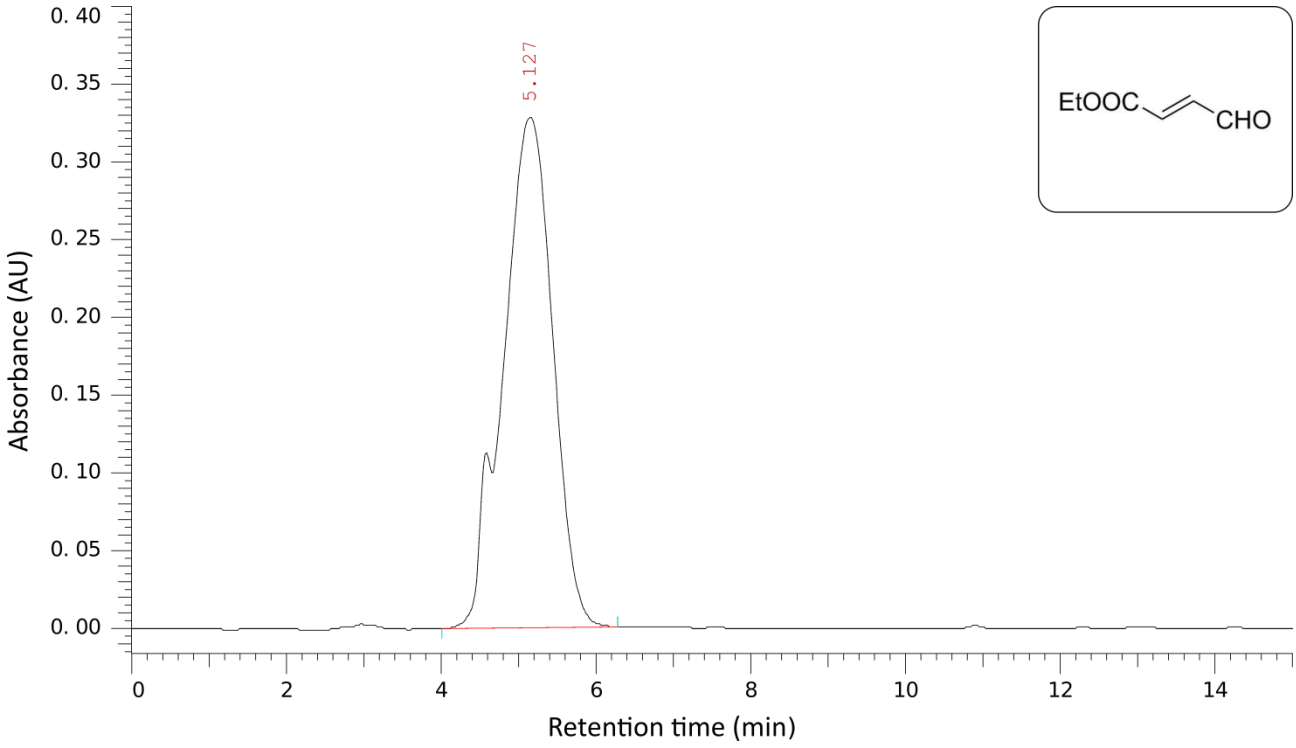


Fig. S109 Chromatogram of ethyl 4-oxobut-2-enoate at 250 nm with the structure in insert. The compound was monitored with Method 2.

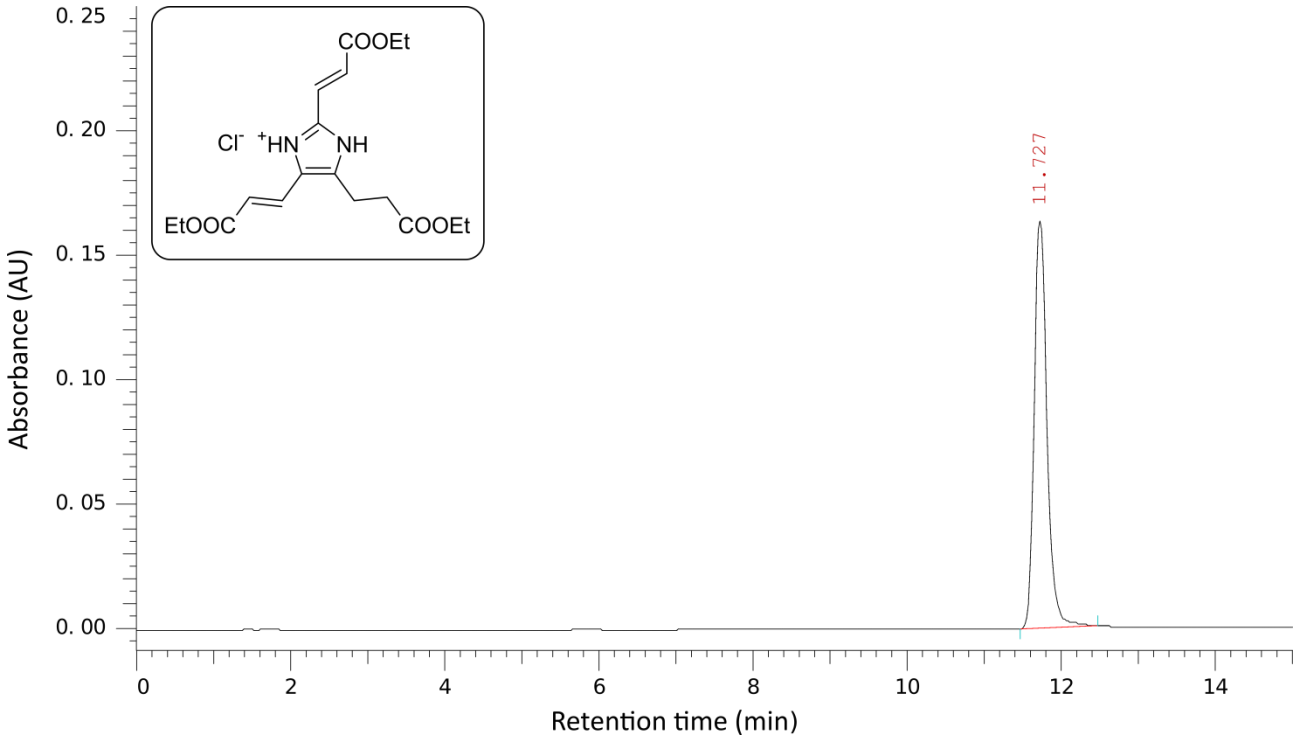


Fig. S110 Chromatogram of **13** at 250 nm with the structure in insert. The compound was monitored with Method 2.

6. Kinetic studies

The fitting of the reaction rate model on the experimental data was performed by varying the [k_1;k_2] vector using the MATLAB[2] Optimisation Tool with *fmincon* solver and interior point algorithm on an objective function which numerically solves the following differential equations and gives the sum of square deviation (SSD) as output:

$$\frac{\mathrm{d[A]}}{\mathrm{d}t} = -3[\mathrm{A}]^n k_1 \quad (1)$$

$$\frac{\mathrm{d[B]}}{\mathrm{d}t} = [\mathrm{A}]^n k_1 - [\mathrm{B}]k_2 \quad (2)$$

$$\frac{\mathrm{d[C]}}{\mathrm{d}t} = [\mathrm{B}]k_2 \quad (3)$$

The derivatives were approximated by the solver. The initial concentrations were $[\mathrm{A}]_0 = 0.5$ mol dm^{-3}, $[\mathrm{B}]_0 = 0$ mol dm^{-3} and $[\mathrm{C}]_0 = 0$ mol dm^{-3}, according to the experimental procedure. The optimisations were run from a suitable starting point using [0;0] lower bound and a suitable upper bound. If any of the obtained optimum values were close to the upper bound, the optimisation was repeated using an extended upper bound. Different *n* values of 1–5 were tested,

and the optimised SSDs are summarized in Table S1. The calculated reaction rate curves were obtained using the optimised [k_1;k_2] values and solving the same differential equations.

Table S1 SSDs on the experimental data for different overall rate orders (n). Fitting with $n = 3$ resulted in the lowest SSD in three out of four cases.

n	Sum of square deviations *p*-Substituent:			
	$-NO_2$	$-SF_5$	$-CF_3$	–COOMe
1	5.67E-03	9.39E-05	4.32E-04	1.24E-03
2	1.12E-03	9.75E-05	4.44E-04	3.73E-04
3	4.82E-04	7.09E-06	1.53E-04	2.16E-04
4	6.29E-04	1.71E-05	3.98E-05	2.51E-04
5	8.10E-04	2.18E-05	5.66E-05	3.36E-04

7. Quantum mechanical calculations

7.1. Computational methods and findings

All calculations were performed using Gaussian 09[3] for Windows (Gaussian Inc., Wallingford, CT), using DFT B3LYP/6-31G(d,p) method. All calculations were run using IEFPCM solvation model and THF as solvent. (Among the available solvents in Gaussian 09, the properties of THF are the closest to the ones of 2-MeTHF). True minima on the potential energy hypersurface were identified by the presence of no imaginary frequencies and transition state structures were confirmed by finding only one imaginary frequency. All enthalpy and Gibbs free energy values reported in the article have been thermally corrected for conditions 298.15 K and 1 atm. The correction factor can be obtained through a frequency calculation using unscaled frequencies. Computational raw data is listed providing standard orientation Cartesian coordinates, electronic energies; zero-point vibrational energies (ZPVE) and standard thermodynamic quantities at 298.15 K and 1.00 atm. NMR calculations were performed using the Gauge-Independent Atomic Orbital (GIAO) method. To determine nuclear independent chemical shifts (NICSs) ghost atoms (Bq) were added to the optimised structures.

Boltzmann population was calculated according to the following equation:

$$\frac{N_2}{N_1} = e^{\frac{\Delta G_1 - \Delta G_2}{kT}} \quad (4)$$

Where N_1 and N_2, and ΔG_1 and ΔG_2 (J) are the populations and relative DFT (B3LYP/6-31G(d,p)) Gibbs free energies of two conformers. T (K) is the absolute temperature and k is the Boltzmann constant ($1.38064852 \cdot 10^{-23}$ J K^{-1}).

HOMO and LUMO orbitals of **1zw** (**Fig. S111** and **Fig. S112**) were visualised to show the orbital symmetries leading to disrotatory (thermal) and conrotatory (UV) cyclizations. The canonical orbitals were generated using 6-31G(d,p) basis set and were visualized at 0.02 isovalue.

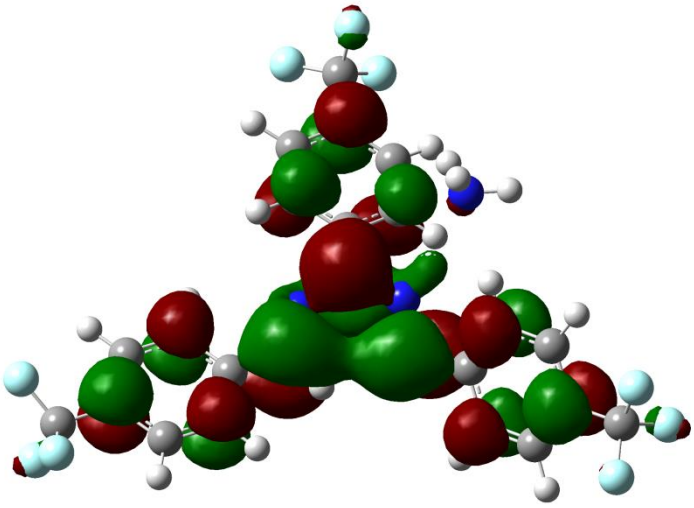


Fig. S111 HOMO orbital of **1zw** visualised to show the lobes on methine carbons with the same signs which leads to disrotatory cyclization under thermal initiation.

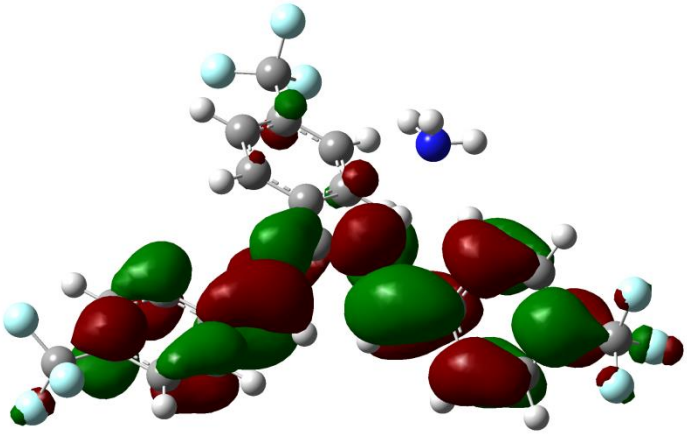
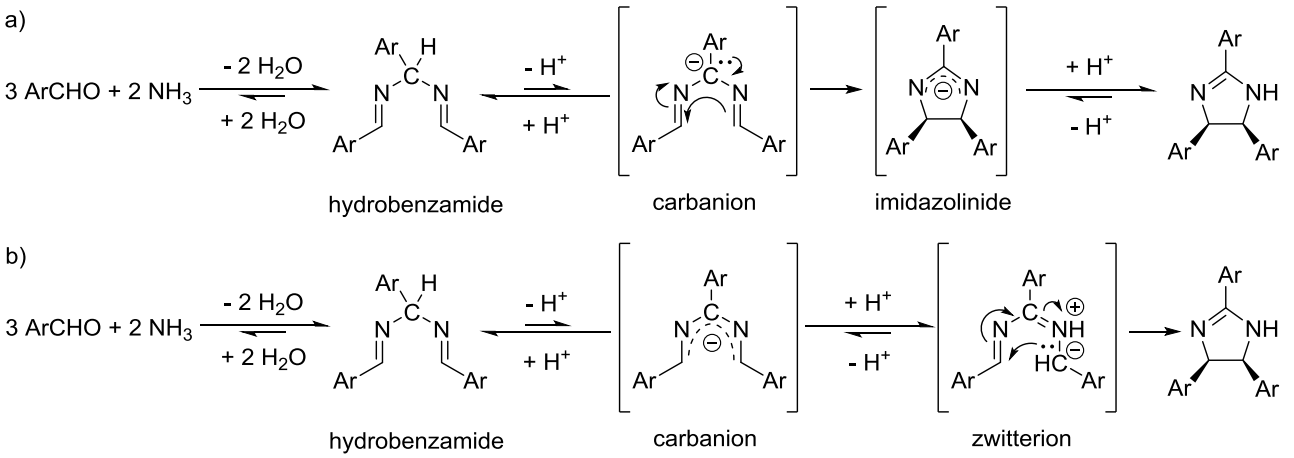
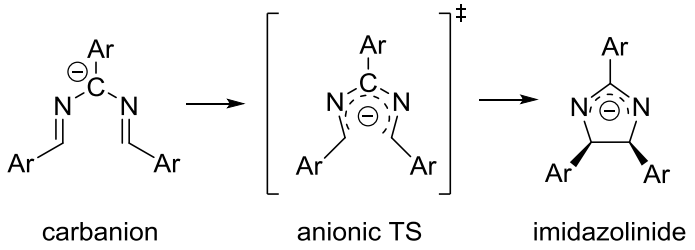


Fig. S112 LUMO orbital of **1zw** visualised to show the lobes on methine carbons with opposite signs which leads to disrotatory cyclization under UV initiation.



Scheme S1 (a) Earlier proposed mechanism of the reaction between aromatic aldehydes[4] and an ammonia source and (b) the mechanism found in this work.

Table S2 Calculated relative DFT (B3LYP/6-31G(d,p)) Gibbs free energies (and enthalpies) of the ring closure from the carbanion intermediate. The results show that this step has relatively high Gibbs free energy barrier compared to the already high energy carbanion intermediate. This and the positive reaction Gibbs free energies for the EWG substituted species suggest that the reaction will not progress via this route.



p-Substituent	ΔG (ΔH) (kJ mol^{-1})		
	Carbanion	Anionic TS	Imidazolinide
$-NO_2$	0.00 (0.00)	78.39 (77.89)	46.16 (40.39)
$-SF_5$	0.00 (0.00)	73.74 (67.03)	21.22 (12.95)
$-CF_3$	0.00 (0.00)	70.50 (64.68)	13.94 (7.43)
–Br	0.00 (0.00)	62.89 (60.75)	3.59 (-2.12)
–H	0.00 (0.00)	64.58 (59.65)	-1.71 (-5.92)

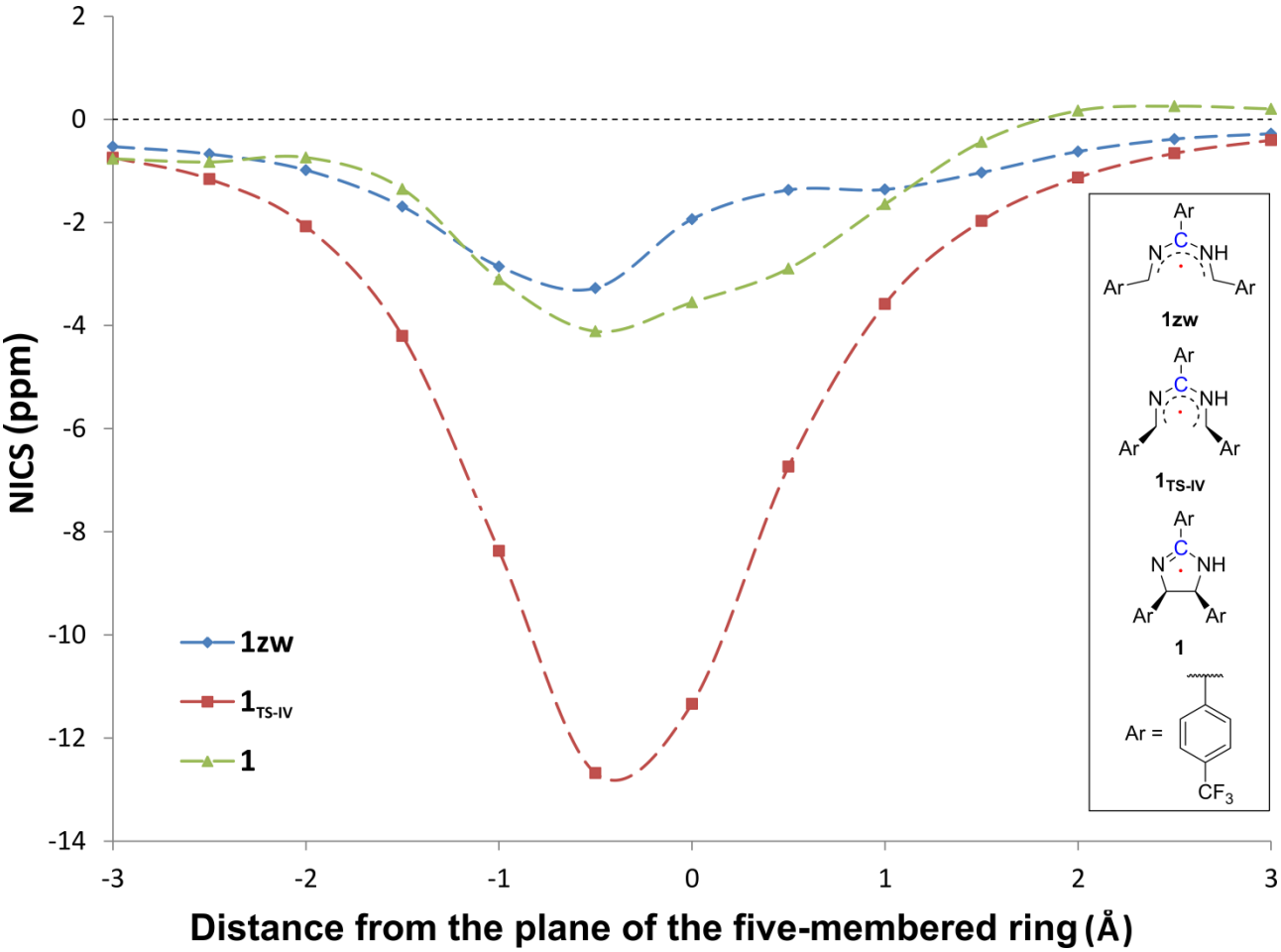
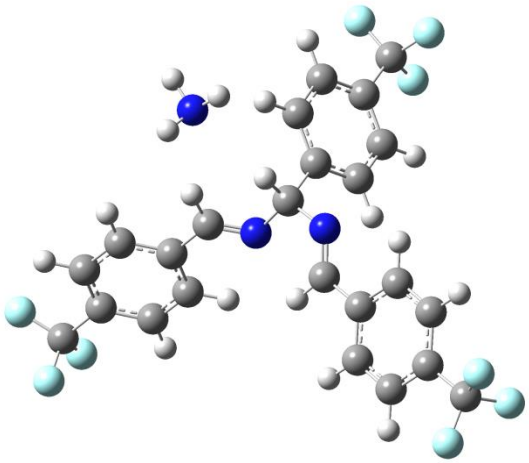


Fig. S113 NICS values calculated in function of distance from the plane if the five-membered ring in **1zw**, $\mathbf{1}_{\mathbf{TS\text{-}IV}}$ and **1**. The ghost atoms for the calculation were placed in the middle of the rings, perpendicularly to it as shown in insert. The red dots illustrate the positions of the 0 Å ghost atoms which were placed 1.19 Å away from the blue carbon atoms.

7.2. Computational raw data

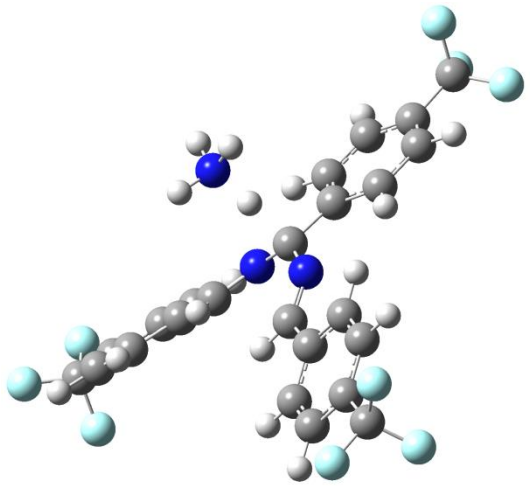
1hb+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5220070.927	kJ·mol^{-1}
Enthalpy (H)	-5218969.621	kJ·mol^{-1}
Gibbs free energy (G)	-5219269.525	kJ·mol^{-1}
ZPVE	1007.588	kJ·mol^{-1}
Correction to U	1098.827	kJ·mol^{-1}
Correction to H	1101.305	kJ·mol^{-1}
Correction to G	801.402	kJ·mol^{-1}
S_{total}	1005.905	J·mol^{-1}·K^{-1}
S_{vib}	654.750	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.701685	-0.705808	0.397212
2	6	0	-1.929551	-0.380814	1.183602
3	6	0	0.064908	0.844864	1.128910
4	1	0	0.913378	-1.357369	0.005654
5	1	0	-2.054434	-0.054943	2.226211
6	7	0	-0.919639	-0.027816	0.484630
7	7	0	1.446254	0.408216	0.966104
8	6	0	-3.002645	-1.235701	0.643025
9	6	0	-4.066033	-1.607577	1.478084
10	6	0	-2.987918	-1.684115	-0.688559
11	6	0	-5.095439	-2.415029	0.999934
12	1	0	-4.087921	-1.259324	2.506713
13	6	0	-4.011557	-2.489603	-1.169822
14	1	0	-2.168461	-1.385787	-1.332751
15	6	0	-5.067399	-2.855891	-0.324820
16	1	0	-5.918223	-2.694144	1.648441
17	1	0	-4.001782	-2.828339	-2.199976
18	6	0	3.084671	-1.191491	0.224910
19	6	0	3.301263	-2.427832	-0.399474
20	6	0	4.190082	-0.447767	0.671800
21	6	0	4.593466	-2.916867	-0.579656
22	1	0	2.451932	-3.010758	-0.744379
23	6	0	5.479840	-0.930794	0.495462
24	1	0	4.016584	0.506357	1.156788
25	6	0	5.682987	-2.167612	-0.131490
26	1	0	4.753608	-3.875676	-1.059498
27	1	0	6.330430	-0.356712	0.846887
28	6	0	-0.098041	2.252781	0.556803
29	6	0	-0.809633	3.215590	1.280270
30	6	0	0.414546	2.580934	-0.703498
31	6	0	-1.002653	4.492712	0.756101
32	1	0	-1.214343	2.956801	2.254949
33	6	0	0.223492	3.854274	-1.233428
34	1	0	0.968765	1.839200	-1.268915
35	6	0	-0.486874	4.811983	-0.502558
36	1	0	-1.556494	5.236054	1.319204
37	1	0	0.618291	4.102816	-2.212606
38	6	0	7.084561	-2.655186	-0.371614
39	6	0	-6.145118	-3.772718	-0.834042
40	6	0	-0.645148	6.202748	-1.047174
41	9	0	-0.700229	6.217454	-2.399309
42	9	0	0.390041	7.007464	-0.695528
43	9	0	-1.769443	6.803278	-0.592668
44	9	0	-5.814016	-5.077567	-0.668379
45	9	0	-6.376723	-3.597871	-2.154830
46	9	0	-7.319130	-3.585840	-0.190142
47	9	0	7.920756	-2.307231	0.633554
48	9	0	7.144091	-3.999877	-0.497903
49	9	0	7.610217	-2.133195	-1.507970
50	1	0	-0.113178	0.906155	2.213250
51	1	0	-1.592856	0.538880	4.976963
52	1	0	-0.675737	1.870191	4.851502
53	1	0	-2.293041	1.997878	4.856309
54	7	0	-1.524836	1.434273	4.496972

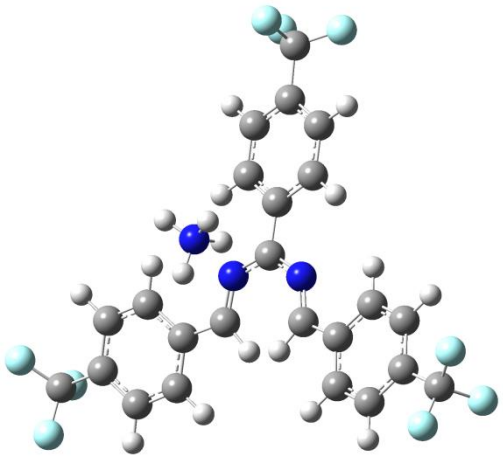
$\mathbf{1}_{TS\text{-}I}$-H-NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5219977.075	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5218889.916	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5219172.237	$kJ \cdot mol^{-1}$
ZPVE	997.782	$kJ \cdot mol^{-1}$
Correction to U	1084.681	$kJ \cdot mol^{-1}$
Correction to H	1087.160	$kJ \cdot mol^{-1}$
Correction to G	804.839	$kJ \cdot mol^{-1}$
S_{total}	946.931	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	595.571	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-1.599537	-0.956260	0.546916
2	6	0	1.465305	-1.057056	0.110236
3	6	0	0.008214	0.823288	0.510132
4	1	0	-0.936686	-1.676999	1.036495
5	1	0	0.672832	-1.779999	-0.099230
6	7	0	1.248991	0.181855	0.386155
7	7	0	-1.252090	0.247635	0.247866
8	6	0	2.828366	-1.594203	0.009480
9	6	0	3.013360	-2.933841	-0.377317
10	6	0	3.967828	-0.819014	0.301144
11	6	0	4.287974	-3.482829	-0.478036
12	1	0	2.146015	-3.548875	-0.601536
13	6	0	5.241170	-1.362319	0.202553
14	1	0	3.832346	0.211269	0.610462
15	6	0	5.407771	-2.698720	-0.186785
16	1	0	4.413578	-4.518571	-0.774304
17	1	0	6.110512	-0.756396	0.435571
18	6	0	-2.962249	-1.448261	0.299784
19	6	0	-3.319512	-2.737892	0.730821
20	6	0	-3.929841	-0.667871	-0.361434
21	6	0	-4.602403	-3.233993	0.519612
22	1	0	-2.583667	-3.353982	1.240725
23	6	0	-5.210889	-1.158533	-0.573734
24	1	0	-3.653976	0.323100	-0.704267
25	6	0	-5.553293	-2.444211	-0.132737
26	1	0	-4.866935	-4.227572	0.864698
27	1	0	-5.951062	-0.547168	-1.078985
28	6	0	0.068723	2.285403	0.191510
29	6	0	-1.112011	3.049517	0.094452
30	6	0	1.296068	2.966682	0.057111
31	6	0	-1.070890	4.420874	-0.133812
32	1	0	-2.067060	2.546905	0.190916
33	6	0	1.340292	4.338279	-0.164014
34	1	0	2.216592	2.399372	0.114867
35	6	0	0.156544	5.078586	-0.264205
36	1	0	-1.995804	4.982391	-0.216021
37	1	0	2.299037	4.835031	-0.276155
38	6	0	-6.918662	-2.995981	-0.420337
39	6	0	6.786983	-3.265886	-0.345160
40	6	0	0.214295	6.561649	-0.447394
41	9	0	1.246657	6.940957	-1.240995
42	9	0	-0.917581	7.060541	-0.999675
43	9	0	0.385648	7.224538	0.730242
44	9	0	7.295015	-3.039419	-1.584386
45	9	0	7.665560	-2.722839	0.531141
46	9	0	6.813838	-4.606655	-0.160210
47	9	0	-7.864097	-2.027576	-0.449990
48	9	0	-7.306418	-3.907549	0.502296
49	9	0	-6.972621	-3.621616	-1.624299
50	1	0	-0.062054	0.919081	1.975445
51	1	0	-0.974613	1.456429	3.521623
52	1	0	0.677380	1.410460	3.616337
53	1	0	-0.190275	0.001310	3.613831
54	7	0	-0.142872	0.944272	3.231649

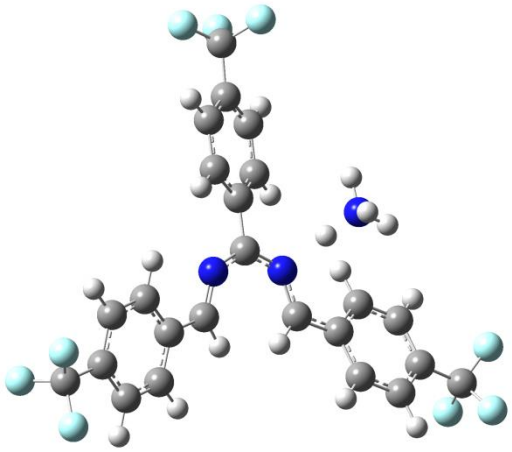
1cU+NH_4^+



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5219995.133	kJ·mol^{-1}
Enthalpy (H)	-5218894.450	kJ·mol^{-1}
Gibbs free energy (G)	-5219183.770	kJ·mol^{-1}
ZPVE	1009.237	kJ·mol^{-1}
Correction to U	1098.205	kJ·mol^{-1}
Correction to H	1100.684	kJ·mol^{-1}
Correction to G	811.363	kJ·mol^{-1}
S_{total}	970.408	J·mol^{-1}·K^{-1}
S_{vib}	619.031	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.544298	-1.158044	-0.166233
2	6	0	-1.580211	-1.103542	-0.389720
3	6	0	0.001592	0.699845	-0.172178
4	1	0	0.814470	-1.966463	-0.125850
5	1	0	-0.882740	-1.864711	-0.738741
6	7	0	-1.247289	0.133539	-0.154012
7	7	0	1.232373	0.107210	-0.210125
8	6	0	-2.966277	-1.548084	-0.276291
9	6	0	-3.300489	-2.876295	-0.612579
10	6	0	-4.001482	-0.700098	0.174940
11	6	0	-4.607805	-3.338371	-0.513656
12	1	0	-2.519882	-3.549417	-0.957247
13	6	0	-5.306941	-1.157798	0.274151
14	1	0	-3.755614	0.320686	0.445633
15	6	0	-5.620114	-2.481912	-0.067268
16	1	0	-4.843353	-4.364359	-0.775552
17	1	0	-6.089799	-0.493411	0.625697
18	6	0	2.935830	-1.594196	-0.119520
19	6	0	3.228268	-2.970583	-0.013934
20	6	0	4.021898	-0.692753	-0.181688
21	6	0	4.539382	-3.429356	0.032876
22	1	0	2.410226	-3.684729	0.034763
23	6	0	5.331182	-1.147483	-0.135554
24	1	0	3.813364	0.367548	-0.269244
25	6	0	5.601112	-2.519898	-0.024745
26	1	0	4.741328	-4.491539	0.120795
27	1	0	6.152619	-0.439410	-0.179667
28	6	0	0.012739	2.181037	-0.199584
29	6	0	1.224122	2.911742	-0.199654
30	6	0	-1.187431	2.929788	-0.217418
31	6	0	1.235175	4.299844	-0.205594
32	1	0	2.158339	2.364086	-0.201168
33	6	0	-1.177299	4.318747	-0.215094
34	1	0	-2.130046	2.397421	-0.245143
35	6	0	0.034004	5.020869	-0.209666
36	1	0	2.182338	4.830246	-0.213697
37	1	0	-2.115966	4.863488	-0.233996
38	6	0	7.016239	-3.007504	-0.033395
39	6	0	-7.040129	-2.953419	-0.010695
40	6	0	0.048320	6.512898	-0.143833
41	9	0	-1.053135	7.067434	-0.706705
42	9	0	1.127533	7.047806	-0.766964
43	9	0	0.089226	6.978044	1.137566
44	9	0	-7.723333	-2.675243	-1.152957
45	9	0	-7.734067	-2.367236	0.995782
46	9	0	-7.130713	-4.292762	0.169338
47	9	0	7.859216	-2.141861	0.581867
48	9	0	7.151766	-4.204755	0.585993
49	9	0	7.500411	-3.173592	-1.293474
50	1	0	-0.008515	0.721808	1.779969
51	1	0	0.784324	1.023472	3.251504
52	1	0	-0.880668	1.078595	3.188061
53	1	0	-0.089515	-0.383302	3.060407
54	7	0	-0.047789	0.610232	2.826632

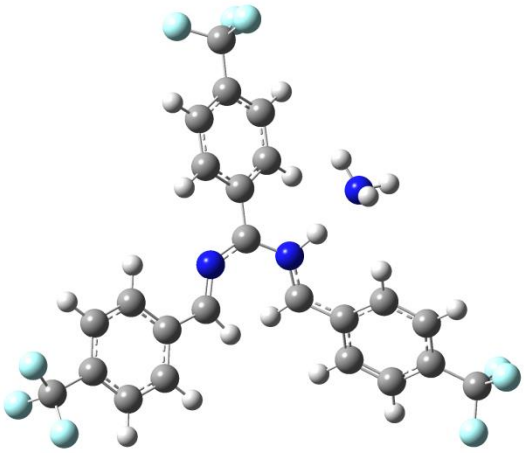
1cU-H-NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5220021.741	kJ·mol^{-1}
Enthalpy (H)	-5218924.960	kJ·mol^{-1}
Gibbs free energy (G)	-5219205.097	kJ·mol^{-1}
ZPVE	1007.752	kJ·mol^{-1}
Correction to U	1094.303	kJ·mol^{-1}
Correction to H	1096.781	kJ·mol^{-1}
Correction to G	816.644	kJ·mol^{-1}
S_{total}	939.609	J·mol^{-1}·K^{-1}
S_{vib}	588.216	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.468193	-1.157487	-0.130143
2	6	0	-1.647605	-1.155559	-0.326667
3	6	0	-0.103085	0.684992	-0.148108
4	1	0	0.722700	-1.943157	-0.091210
5	1	0	-0.951898	-1.923099	-0.664994
6	7	0	-1.320859	0.086668	-0.111393
7	7	0	1.139480	0.125957	-0.142417
8	6	0	-3.031702	-1.603997	-0.207177
9	6	0	-3.350688	-2.949072	-0.484623
10	6	0	-4.076740	-0.742471	0.190780
11	6	0	-4.655453	-3.416505	-0.377637
12	1	0	-2.560623	-3.631485	-0.786845
13	6	0	-5.379538	-1.205718	0.298166
14	1	0	-3.841324	0.292661	0.410513
15	6	0	-5.678123	-2.547136	0.016521
16	1	0	-4.880862	-4.455535	-0.592546
17	1	0	-6.171546	-0.531864	0.608486
18	6	0	2.847671	-1.592679	-0.096508
19	6	0	3.147764	-2.924118	0.281757
20	6	0	3.934813	-0.760406	-0.464814
21	6	0	4.454844	-3.384625	0.330463
22	1	0	2.335070	-3.591279	0.555087
23	6	0	5.243644	-1.221201	-0.413099
24	1	0	3.736940	0.238420	-0.840248
25	6	0	5.517104	-2.533090	-0.004947
26	1	0	4.658353	-4.404327	0.640483
27	1	0	6.058958	-0.566480	-0.702895
28	6	0	-0.133537	2.161199	-0.143820
29	6	0	0.935778	2.927998	-0.664192
30	6	0	-1.252659	2.870311	0.347967
31	6	0	0.907041	4.318505	-0.654396
32	1	0	1.778644	2.419233	-1.120625
33	6	0	-1.282781	4.257733	0.360946
34	1	0	-2.096779	2.306183	0.725404
35	6	0	-0.200790	4.997406	-0.135351
36	1	0	1.735062	4.878450	-1.077096
37	1	0	-2.152049	4.774015	0.755252
38	6	0	6.921374	-3.049434	-0.005861
39	6	0	-7.095911	-3.026302	0.076355
40	6	0	-0.206050	6.491007	-0.063228
41	9	0	-1.457932	7.005071	-0.116044
42	9	0	0.503321	7.058316	-1.069323
43	9	0	0.344789	6.955255	1.093112
44	9	0	-7.762150	-2.810151	-1.089258
45	9	0	-7.809175	-2.396155	1.041110
46	9	0	-7.179926	-4.355692	0.320939
47	9	0	7.830271	-2.063664	0.190499
48	9	0	7.123797	-3.979346	0.959303
49	9	0	7.255688	-3.646207	-1.181246
50	1	0	2.089533	0.944372	0.760578
51	1	0	3.648953	1.112259	1.571090
52	1	0	2.703901	2.471567	1.379856
53	1	0	2.270130	1.305422	2.476657
54	7	0	2.692421	1.467614	1.561942

1zw+NH_3

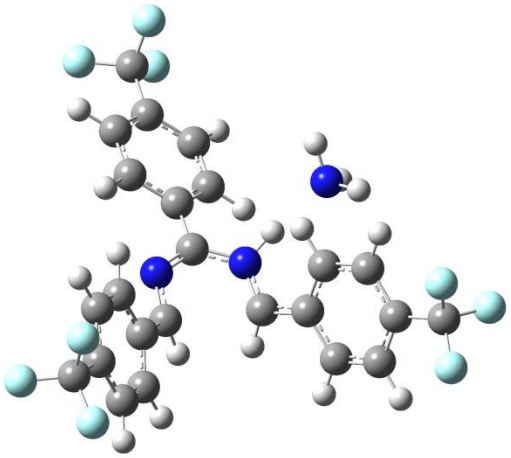


Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5220055.543	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5218954.160	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5219235.743	$kJ \cdot mol^{-1}$
ZPVE	1011.302	$kJ \cdot mol^{-1}$
Correction to U	1098.905	$kJ \cdot mol^{-1}$
Correction to H	1101.383	$kJ \cdot mol^{-1}$
Correction to G	819.800	$kJ \cdot mol^{-1}$
S_{total}	944.459	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	593.074	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.686837	-0.486088	-0.769679
2	6	0	-1.254027	-1.183256	-0.477004
3	6	0	-0.203306	0.976772	-0.320462
4	1	0	1.124618	-0.991777	-1.541382
5	1	0	-0.375016	-1.787871	-0.705586
6	7	0	-1.231724	0.115181	-0.365036
7	7	0	1.135618	0.621917	-0.263408
8	6	0	-2.484216	-1.936343	-0.267224
9	6	0	-2.448023	-3.345042	-0.316831
10	6	0	-3.724308	-1.309717	-0.020512
11	6	0	-3.599090	-4.100019	-0.125323
12	1	0	-1.502145	-3.847200	-0.500839
13	6	0	-4.875527	-2.061103	0.164907
14	1	0	-3.764015	-0.227111	0.017118
15	6	0	-4.819906	-3.461202	0.117186
16	1	0	-3.550968	-5.183224	-0.157969
17	1	0	-5.821895	-1.566461	0.355995
18	6	0	2.998191	-0.988167	-0.463139
19	6	0	3.518859	-2.021184	-1.281870
20	6	0	3.797733	-0.530040	0.610987
21	6	0	4.780242	-2.549068	-1.056746
22	1	0	2.918680	-2.401947	-2.102932
23	6	0	5.062346	-1.058235	0.830390
24	1	0	3.416989	0.230438	1.281118
25	6	0	5.563982	-2.067991	0.000626
26	1	0	5.157881	-3.340322	-1.695317
27	1	0	5.658816	-0.698219	1.661559
28	6	0	-0.509785	2.408849	-0.258446
29	6	0	0.416476	3.384102	-0.687108
30	6	0	-1.768774	2.854351	0.200153
31	6	0	0.115760	4.741245	-0.618926
32	1	0	1.367816	3.076888	-1.108378
33	6	0	-2.073237	4.206292	0.257568
34	1	0	-2.496950	2.117623	0.516818
35	6	0	-1.130090	5.161726	-0.145488
36	1	0	0.839296	5.472527	-0.962812
37	1	0	-3.045405	4.525842	0.618071
38	6	0	6.950489	-2.599623	0.204780
39	6	0	-6.074481	-4.268576	0.261858
40	6	0	-1.439024	6.622166	-0.018168
41	9	0	-2.751629	6.887018	-0.220077
42	9	0	-0.737334	7.374666	-0.898007
43	9	0	-1.140671	7.102076	1.218746
44	9	0	-6.671247	-4.508420	-0.935545
45	9	0	-6.998758	-3.644667	1.029848
46	9	0	-5.841539	-5.480582	0.819445
47	9	0	7.370038	-2.460618	1.483608
48	9	0	7.042497	-3.913707	-0.108966
49	9	0	7.862499	-1.957901	-0.571607
50	1	0	1.722430	1.252643	0.335030
51	1	0	2.404251	2.135591	2.603170
52	1	0	3.415895	2.753453	1.486606
53	1	0	1.878988	3.281616	1.572489
54	7	0	2.456581	2.445423	1.634306

$\mathbf{1}_{TS\text{-}IV}$+$NH_3$

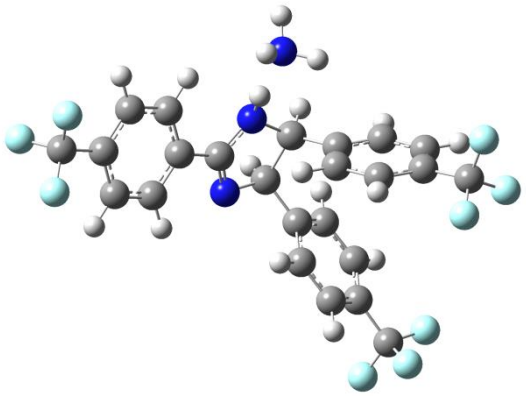
Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5220038.012	kJ·mol^{-1}
Enthalpy (H)	-5218939.450	kJ·mol^{-1}
Gibbs free energy (G)	-5219214.023	kJ·mol^{-1}
ZPVE	1010.471	kJ·mol^{-1}
Correction to U	1096.084	kJ·mol^{-1}
Correction to H	1098.562	kJ·mol^{-1}
Correction to G	823.989	kJ·mol^{-1}
S_{total}	920.949	J·mol^{-1}·K^{-1}
S_{vib}	571.195	J·mol^{-1}·K^{-1}



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	0.206813	1.183850	-1.550651
2	6	0	0.271031	-1.352178	-1.446905
3	6	0	-1.658532	-0.196886	-0.878179
4	1	0	0.341626	0.945957	-2.595698
5	1	0	0.426988	-1.017812	-2.463706
6	7	0	-0.945352	-1.303621	-0.896972
7	7	0	-1.061990	1.031574	-1.029476
8	6	0	1.295446	-2.242089	-0.913036
9	6	0	2.475668	-2.471252	-1.646702
10	6	0	1.153022	-2.867982	0.342787
11	6	0	3.476182	-3.299521	-1.151640
12	1	0	2.605967	-1.990299	-2.612070
13	6	0	2.147213	-3.701285	0.835873
14	1	0	0.252369	-2.687638	0.919267
15	6	0	3.315319	-3.918182	0.092451
16	1	0	4.381207	-3.464302	-1.725468
17	1	0	2.028196	-4.175781	1.804447
18	6	0	1.153426	2.093943	-0.957176
19	6	0	2.219588	2.603811	-1.737811
20	6	0	1.101363	2.472685	0.406758
21	6	0	3.164439	3.461038	-1.194965
22	1	0	2.293802	2.317938	-2.783188
23	6	0	2.042487	3.338914	0.946541
24	1	0	0.330641	2.057799	1.047080
25	6	0	3.080593	3.840935	0.151621
26	1	0	3.972487	3.838110	-1.812836
27	1	0	1.988498	3.609450	1.995831
28	6	0	-3.089307	-0.245788	-0.524171
29	6	0	-3.961318	0.800076	-0.867900
30	6	0	-3.608886	-1.368508	0.146858
31	6	0	-5.309694	0.742640	-0.522387
32	1	0	-3.589831	1.649292	-1.429286
33	6	0	-4.952102	-1.427181	0.491123
34	1	0	-2.942107	-2.186453	0.392540
35	6	0	-5.807956	-0.368632	0.159548
36	1	0	-5.975974	1.551254	-0.800977
37	1	0	-5.341095	-2.296111	1.010944
38	6	0	4.064314	4.815011	0.720726
39	6	0	4.362698	-4.853939	0.619591
40	6	0	-7.248483	-0.417216	0.581303
41	9	0	-7.752328	-1.671715	0.520503
42	9	0	-8.034701	0.370254	-0.187087
43	9	0	-7.413511	0.000780	1.862334
44	9	0	4.042906	-6.155035	0.396009
45	9	0	4.525367	-4.729349	1.958820
46	9	0	5.571243	-4.649579	0.048197
47	9	0	4.252328	4.637425	2.050268
48	9	0	5.278534	4.721933	0.127564
49	9	0	3.663799	6.105989	0.563556
50	1	0	-1.470948	1.822961	-0.480812
51	1	0	-2.629326	3.146789	1.248918
52	1	0	-1.380412	3.984247	0.619736
53	1	0	-2.795081	3.899880	-0.183674
54	7	0	-2.144041	3.355593	0.378670

1+NH_3

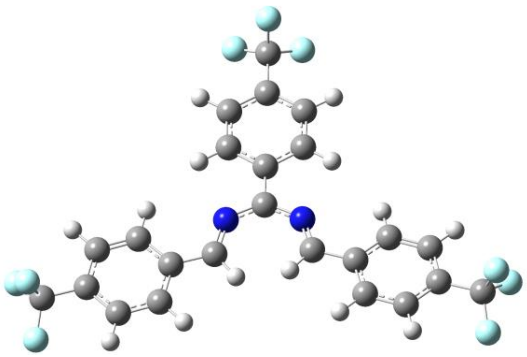
Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5220157.368	kJ·mol^{-1}
Enthalpy (H)	-5219050.448	kJ·mol^{-1}
Gibbs free energy (G)	-5219332.512	kJ·mol^{-1}
ZPVE	1018.012	kJ·mol^{-1}
Correction to U	1104.441	kJ·mol^{-1}
Correction to H	1106.920	kJ·mol^{-1}
Correction to G	824.856	kJ·mol^{-1}
S_{total}	946.069	J·mol^{-1}·K^{-1}
S_{vib}	598.630	J·mol^{-1}·K^{-1}



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	0.176429	-1.285875	1.741835
2	6	0	0.086484	0.268407	2.088599
3	6	0	-1.831691	-0.570788	1.140037
4	1	0	0.096173	-1.815949	2.702441
5	1	0	0.367452	0.411774	3.136098
6	7	0	-1.352829	0.472757	1.902999
7	1	0	-1.706529	1.437160	1.793984
8	7	0	-1.036777	-1.579237	0.969869
9	6	0	0.946347	1.196338	1.243621
10	6	0	2.180105	1.637648	1.739856
11	6	0	0.551804	1.614226	-0.034974
12	6	0	3.005143	2.465842	0.982578
13	1	0	2.500257	1.330284	2.731487
14	6	0	1.368884	2.444261	-0.798981
15	1	0	-0.403058	1.293993	-0.437680
16	6	0	2.599736	2.869951	-0.291892
17	1	0	3.959068	2.795632	1.379532
18	1	0	1.055087	2.753657	-1.790051
19	6	0	1.454765	-1.749113	1.075713
20	6	0	2.580306	-2.050250	1.853642
21	6	0	1.544537	-1.876612	-0.315509
22	6	0	3.773205	-2.456768	1.260380
23	1	0	2.523719	-1.969354	2.935936
24	6	0	2.731530	-2.286667	-0.917640
25	1	0	0.670910	-1.662234	-0.920761
26	6	0	3.850273	-2.573580	-0.130055
27	1	0	4.639024	-2.682432	1.873187
28	1	0	2.791506	-2.378207	-1.996944
29	6	0	-3.205357	-0.542467	0.584924
30	6	0	-3.576409	-1.496763	-0.375185
31	6	0	-4.147049	0.408667	1.002889
32	6	0	-4.856934	-1.494286	-0.914975
33	1	0	-2.845169	-2.232426	-0.688959
34	6	0	-5.432311	0.411984	0.465082
35	1	0	-3.881615	1.146141	1.751539
36	6	0	-5.787376	-0.536602	-0.496056
37	1	0	-5.133332	-2.227460	-1.664668
38	1	0	-6.155183	1.152242	0.789342
39	6	0	5.110962	-3.068724	-0.777514
40	6	0	3.454818	3.811204	-1.090769
41	6	0	-7.188623	-0.566261	-1.039525
42	9	0	-7.760734	0.659587	-1.037490
43	9	0	-7.997258	-1.372388	-0.307571
44	9	0	-7.230070	-1.028542	-2.310006
45	9	0	3.150808	5.110756	-0.839507
46	9	0	3.300567	3.632450	-2.422879
47	9	0	4.770551	3.664346	-0.813918
48	9	0	5.304138	-2.519613	-1.999752
49	9	0	6.209515	-2.794306	-0.036454
50	9	0	5.095659	-4.414119	-0.960577
51	1	0	-2.889831	3.607299	1.046015
52	1	0	-2.389790	3.769562	2.585566
53	1	0	-1.307796	3.793759	1.370131
54	7	0	-2.155671	3.333680	1.695804

1cU

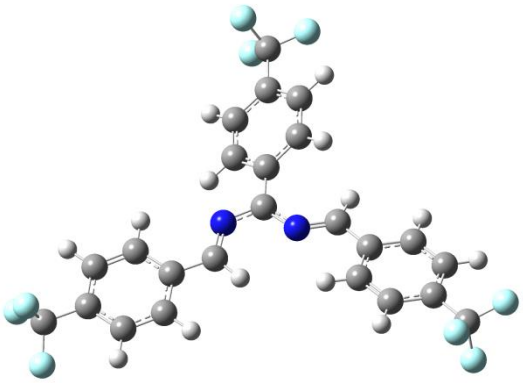
Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5070269.258	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5069312.753	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5069572.215	$kJ \cdot mol^{-1}$
ZPVE	875.762	$kJ \cdot mol^{-1}$
Correction to U	954.024	$kJ \cdot mol^{-1}$
Correction to H	956.505	$kJ \cdot mol^{-1}$
Correction to G	697.043	$kJ \cdot mol^{-1}$
S_{total}	870.255	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	519.490	$J \cdot mol^{-1} \cdot K^{-1}$



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-1.545728	-1.112287	-0.241792
2	6	0	1.543162	-1.114246	0.147907
3	6	0	-0.000602	0.718812	-0.042847
4	1	0	-0.817023	-1.897401	-0.444196
5	1	0	0.812992	-1.901049	0.337679
6	7	0	1.230956	0.144408	-0.019823
7	7	0	-1.232551	0.145006	-0.066404
8	6	0	2.929535	-1.551568	0.171827
9	6	0	3.232243	-2.905395	0.444477
10	6	0	4.013158	-0.678556	-0.085648
11	6	0	4.542682	-3.363587	0.471915
12	1	0	2.418753	-3.600170	0.637605
13	6	0	5.322179	-1.133525	-0.058638
14	1	0	3.797122	0.359333	-0.312919
15	6	0	5.601015	-2.481325	0.218809
16	1	0	4.749018	-4.407915	0.682598
17	1	0	6.138386	-0.447693	-0.263327
18	6	0	-2.932089	-1.550388	-0.253592
19	6	0	-3.237642	-2.901703	-0.534062
20	6	0	-4.013131	-0.678572	0.019521
21	6	0	-4.548295	-3.360787	-0.547162
22	1	0	-2.426827	-3.593170	-0.749084
23	6	0	-5.321851	-1.134091	0.006014
24	1	0	-3.794921	0.359680	0.243109
25	6	0	-5.603728	-2.479972	-0.279286
26	1	0	-4.757651	-4.401410	-0.772077
27	1	0	-6.136730	-0.446918	0.212343
28	6	0	-0.000550	2.194345	-0.037432
29	6	0	-1.203773	2.937637	-0.092079
30	6	0	1.203463	2.936892	0.019573
31	6	0	-1.205271	4.325726	-0.081704
32	1	0	-2.140276	2.396793	-0.148966
33	6	0	1.205245	4.324528	0.020331
34	1	0	2.140051	2.395032	0.064145
35	6	0	-0.000020	5.038702	-0.030370
36	1	0	-2.147241	4.863643	-0.127280
37	1	0	2.148450	4.861445	0.058006
38	6	0	-7.011258	-2.976641	-0.224308
39	6	0	7.014987	-2.954033	0.308783
40	6	0	0.002293	6.527990	0.040257
41	9	0	1.088537	7.075202	-0.564751
42	9	0	0.019529	6.998208	1.321319
43	9	0	-1.093308	7.079336	-0.541074
44	9	0	7.538803	-2.805823	1.558244
45	9	0	7.842320	-2.273305	-0.523394
46	9	0	7.141205	-4.270309	0.005826
47	9	0	-7.902865	-2.049818	-0.657982
48	9	0	-7.198346	-4.090151	-0.975037
49	9	0	-7.402463	-3.304434	1.039405

1cS

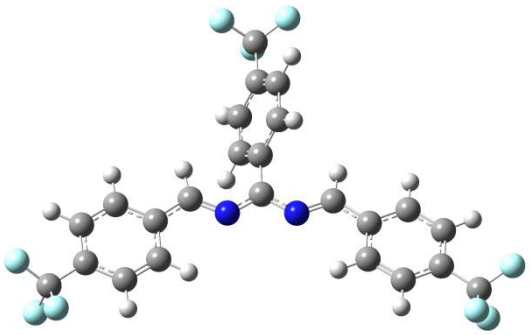
Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5070266.680	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5069310.556	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5069570.190	$kJ \cdot mol^{-1}$
ZPVE	875.497	$kJ \cdot mol^{-1}$
Correction to U	953.646	$kJ \cdot mol^{-1}$
Correction to H	956.124	$kJ \cdot mol^{-1}$
Correction to G	696.489	$kJ \cdot mol^{-1}$
S_{total}	870.845	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	520.042	$J \cdot mol^{-1} \cdot K^{-1}$



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-1.357628	-1.131953	-0.042978
2	6	0	2.273650	0.627091	-0.162004
3	6	0	-0.104326	0.863078	-0.007031
4	1	0	-0.455912	-1.750852	-0.075988
5	1	0	2.483595	1.666400	-0.432959
6	7	0	1.062062	0.175104	0.036523
7	7	0	-1.285643	0.172720	-0.019146
8	6	0	3.430897	-0.242898	-0.089755
9	6	0	4.717223	0.269160	-0.381464
10	6	0	3.339476	-1.608016	0.278116
11	6	0	5.848122	-0.533529	-0.319008
12	1	0	4.818576	1.315210	-0.659575
13	6	0	4.467029	-2.410506	0.339058
14	1	0	2.362672	-2.012994	0.517538
15	6	0	5.734828	-1.882210	0.044316
16	1	0	6.823892	-0.115514	-0.544416
17	1	0	4.374344	-3.452984	0.627645
18	6	0	-2.626914	-1.828789	-0.022484
19	6	0	-2.653309	-3.242346	-0.082553
20	6	0	-3.872495	-1.156481	0.048667
21	6	0	-3.849544	-3.946623	-0.077299
22	1	0	-1.712916	-3.784544	-0.139541
23	6	0	-5.067273	-1.857917	0.051204
24	1	0	-3.871842	-0.073423	0.101769
25	6	0	-5.070175	-3.261273	-0.014822
26	1	0	-3.842282	-5.030496	-0.130743
27	1	0	-6.009832	-1.321129	0.099004
28	6	0	-0.248364	2.330369	-0.017452
29	6	0	-1.409181	2.926873	-0.570053
30	6	0	0.701655	3.207588	0.557683
31	6	0	-1.597970	4.300489	-0.568764
32	1	0	-2.159118	2.278790	-1.007208
33	6	0	0.512226	4.585171	0.567175
34	1	0	1.583788	2.805920	1.040416
35	6	0	-0.632239	5.148474	-0.006968
36	1	0	-2.490968	4.723389	-1.018839
37	1	0	1.257665	5.226709	1.026200
38	6	0	-6.357097	-4.014222	0.051246
39	6	0	6.936506	-2.767786	0.055799
40	6	0	-0.861902	6.622871	0.041017
41	9	0	0.295333	7.326679	0.110565
42	9	0	-1.599149	7.004966	1.122077
43	9	0	-1.537794	7.076642	-1.045380
44	9	0	7.129494	-3.408428	-1.132129
45	9	0	6.848123	-3.746198	0.992291
46	9	0	8.082910	-2.085349	0.301368
47	9	0	-7.379216	-3.344953	-0.540415
48	9	0	-6.278302	-5.228749	-0.548105
49	9	0	-6.763749	-4.255068	1.330506

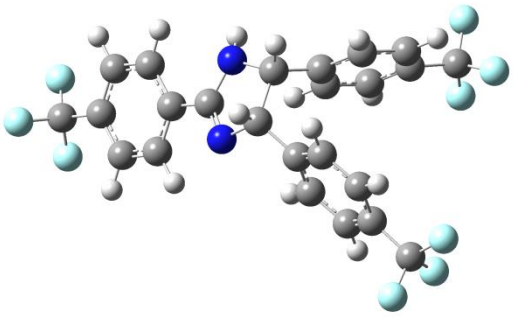
1cW

Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5070254.306	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5069299.067	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5069562.889	$kJ \cdot mol^{-1}$
ZPVE	874.029	$kJ \cdot mol^{-1}$
Correction to U	952.761	$kJ \cdot mol^{-1}$
Correction to H	955.239	$kJ \cdot mol^{-1}$
Correction to G	691.417	$kJ \cdot mol^{-1}$
S_{total}	884.887	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	534.171	$J \cdot mol^{-1} \cdot K^{-1}$



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	2.343147	0.123899	-0.074316
2	6	0	-2.366242	0.165929	0.013039
3	6	0	-0.008750	0.363254	-0.025948
4	1	0	2.540754	1.200801	-0.115652
5	1	0	-2.547089	1.245233	0.066747
6	7	0	-1.156928	-0.347150	-0.034153
7	7	0	1.125637	-0.369982	-0.032480
8	6	0	-3.540727	-0.674485	0.009353
9	6	0	-4.831325	-0.094581	0.088078
10	6	0	-3.469399	-2.089037	-0.075737
11	6	0	-5.978643	-0.874434	0.089109
12	1	0	-4.920081	0.987392	0.147703
13	6	0	-4.614603	-2.867733	-0.073836
14	1	0	-2.490158	-2.549764	-0.145452
15	6	0	-5.884609	-2.271228	0.006269
16	1	0	-6.954596	-0.402685	0.147380
17	1	0	-4.533117	-3.948201	-0.143436
18	6	0	3.504874	-0.733947	-0.078805
19	6	0	4.803161	-0.172788	-0.161802
20	6	0	3.412779	-2.148031	-0.002668
21	6	0	5.939394	-0.969176	-0.168930
22	1	0	4.907106	0.907590	-0.225511
23	6	0	4.546484	-2.942861	-0.010476
24	1	0	2.426742	-2.595106	0.060451
25	6	0	5.824979	-2.364543	-0.096284
26	1	0	6.921374	-0.512293	-0.239252
27	1	0	4.448877	-4.023093	0.043571
28	6	0	0.006224	1.860861	-0.005599
29	6	0	0.580336	2.566075	1.067968
30	6	0	-0.557422	2.609089	-1.055181
31	6	0	0.594754	3.957953	1.094663
32	1	0	1.014866	2.012214	1.894359
33	6	0	-0.548461	4.001320	-1.037506
34	1	0	-1.007067	2.089201	-1.895421
35	6	0	0.027923	4.681108	0.040262
36	1	0	1.033269	4.482593	1.937070
37	1	0	-0.990049	4.559495	-1.856518
38	6	0	7.041957	-3.223529	-0.037058
39	6	0	-7.112342	-3.113853	0.077282
40	6	0	0.093329	6.178728	0.035237
41	9	0	-0.952921	6.736443	-0.619997
42	9	0	1.215619	6.641504	-0.576612
43	9	0	0.102446	6.696327	1.286805
44	9	0	-7.454302	-3.446548	1.356079
45	9	0	-6.974654	-4.291043	-0.584505
46	9	0	-8.200901	-2.490974	-0.443529
47	9	0	6.859601	-4.424211	-0.645113
48	9	0	8.119090	-2.641984	-0.623284
49	9	0	7.425029	-3.513708	1.240400

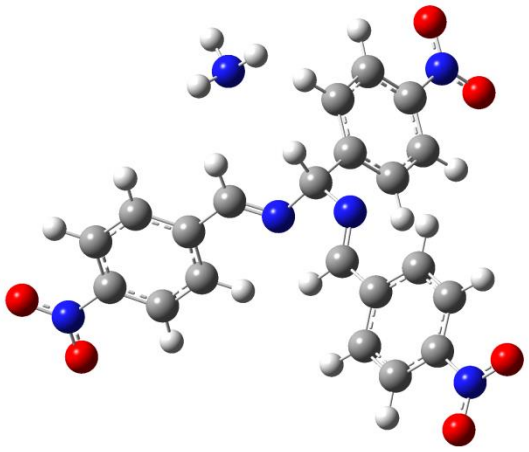
1



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5071624.701	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5070624.165	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5070878.945	$kJ \cdot mol^{-1}$
ZPVE	921.936	$kJ \cdot mol^{-1}$
Correction to U	998.056	$kJ \cdot mol^{-1}$
Correction to H	1000.537	$kJ \cdot mol^{-1}$
Correction to G	745.756	$kJ \cdot mol^{-1}$
S_{total}	854.553	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	507.979	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	0.075437	-1.165024	1.844070
2	6	0	0.053944	0.392907	2.182696
3	6	0	-1.914878	-0.382241	1.256223
4	1	0	-0.015302	-1.686995	2.807127
5	1	0	0.356610	0.531757	3.223694
6	7	0	-1.386444	0.643771	2.031133
7	1	0	-1.675664	1.593903	1.832184
8	7	0	-1.160013	-1.414964	1.090113
9	6	0	0.921285	1.287572	1.313486
10	6	0	2.165817	1.714851	1.795317
11	6	0	0.524194	1.690922	0.031300
12	6	0	2.998361	2.516807	1.019433
13	1	0	2.487348	1.417237	2.789241
14	6	0	1.349085	2.496701	-0.750501
15	1	0	-0.434833	1.376306	-0.366904
16	6	0	2.589349	2.909221	-0.257949
17	1	0	3.960718	2.836133	1.404439
18	1	0	1.033053	2.797406	-1.743215
19	6	0	1.323162	-1.682070	1.159863
20	6	0	2.447401	-2.024433	1.922360
21	6	0	1.384670	-1.818613	-0.231789
22	6	0	3.612880	-2.481188	1.311722
23	1	0	2.412151	-1.937267	3.005019
24	6	0	2.544173	-2.279882	-0.850619
25	1	0	0.512106	-1.570945	-0.825859
26	6	0	3.662408	-2.607989	-0.079129
27	1	0	4.478862	-2.738592	1.911616
28	1	0	2.582732	-2.379115	-1.930092
29	6	0	-3.284454	-0.281349	0.706703
30	6	0	-3.677159	-1.152269	-0.321278
31	6	0	-4.199306	0.664538	1.191015
32	6	0	-4.954683	-1.072014	-0.861995
33	1	0	-2.966635	-1.883393	-0.688794
34	6	0	-5.480871	0.746270	0.651133
35	1	0	-3.924994	1.326807	2.005149
36	6	0	-5.857691	-0.118837	-0.378003
37	1	0	-5.248621	-1.739787	-1.664078
38	1	0	-6.182535	1.481705	1.028144
39	6	0	4.892890	-3.159364	-0.740115
40	6	0	3.459194	3.823784	-1.073049
41	6	0	-7.256460	-0.065590	-0.928206
42	9	0	-7.786792	1.175456	-0.846033
43	9	0	-8.093842	-0.891798	-0.254380
44	9	0	-7.303983	-0.439793	-2.226627
45	9	0	3.235238	5.129871	-0.779719
46	9	0	3.243386	3.683154	-2.400623
47	9	0	4.775146	3.601206	-0.852434
48	9	0	5.069978	-2.659146	-1.984982
49	9	0	6.015859	-2.888880	-0.035032
50	9	0	4.836923	-4.509239	-0.872797

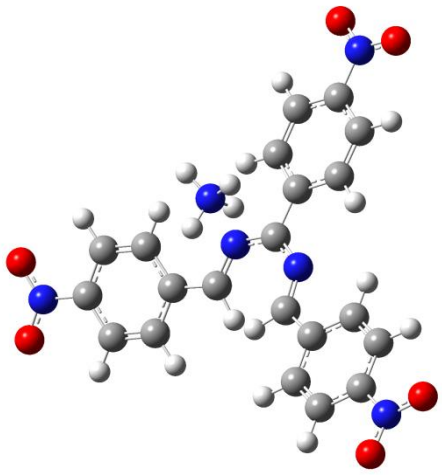
3hb+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-4176196.408	kJ·mol^{-1}
Enthalpy (H)	-4175120.126	kJ·mol^{-1}
Gibbs free energy (G)	-4175393.923	kJ·mol^{-1}
ZPVE	991.501	kJ·mol^{-1}
Correction to U	1073.801	kJ·mol^{-1}
Correction to H	1076.282	kJ·mol^{-1}
Correction to G	802.485	kJ·mol^{-1}
S_{total}	918.334	J·mol^{-1}·K^{-1}
S_{vib}	572.447	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.726119	-0.698661	0.311996
2	6	0	-1.910662	-0.399619	1.058966
3	6	0	0.068146	0.850988	0.993057
4	1	0	0.950246	-1.385182	-0.041768
5	1	0	-2.045435	-0.063689	2.096364
6	7	0	-0.903409	-0.042668	0.357999
7	7	0	1.454657	0.435455	0.831247
8	6	0	-2.964955	-1.278233	0.518220
9	6	0	-4.020764	-1.671472	1.355661
10	6	0	-2.932982	-1.728694	-0.813718
11	6	0	-5.030264	-2.503782	0.882981
12	1	0	-4.050646	-1.323151	2.383491
13	6	0	-3.932630	-2.558444	-1.300179
14	1	0	-2.116771	-1.414848	-1.454021
15	6	0	-4.968325	-2.934602	-0.440737
16	1	0	-5.850664	-2.817362	1.515039
17	1	0	-3.926613	-2.914913	-2.322006
18	6	0	3.119833	-1.158522	0.153820
19	6	0	3.361112	-2.425960	-0.399219
20	6	0	4.207039	-0.356323	0.544180
21	6	0	4.660634	-2.894689	-0.563111
22	1	0	2.524771	-3.048659	-0.701955
23	6	0	5.508831	-0.809079	0.387081
24	1	0	4.010034	0.621177	0.968921
25	6	0	5.715942	-2.075815	-0.165887
26	1	0	4.863666	-3.869255	-0.987331
27	1	0	6.358264	-0.206139	0.680748
28	6	0	-0.118216	2.247099	0.400602
29	6	0	-0.843041	3.208500	1.115925
30	6	0	0.392970	2.562496	-0.865246
31	6	0	-1.052604	4.476824	0.582219
32	1	0	-1.240071	2.955246	2.094694
33	6	0	0.191072	3.823985	-1.414199
34	1	0	0.958477	1.820820	-1.418489
35	6	0	-0.530371	4.764740	-0.678131
36	1	0	-1.604869	5.235042	1.122237
37	1	0	0.580390	4.086910	-2.389223
38	1	0	-0.108991	0.924397	2.076583
39	1	0	-1.574505	0.542109	4.783272
40	1	0	-0.669344	1.884096	4.690606
41	1	0	-2.286350	1.990444	4.615754
42	7	0	-1.494505	1.434142	4.298711
43	7	0	-0.744028	6.098230	-1.247202
44	8	0	-0.279210	6.334679	-2.364742
45	8	0	-1.378837	6.919717	-0.581406
46	7	0	7.090013	-2.560018	-0.334221
47	8	0	8.011736	-1.824038	0.024502
48	8	0	7.255139	-3.678668	-0.825608
49	7	0	-6.028323	-3.812334	-0.949968
50	8	0	-6.931947	-4.138254	-0.177496
51	8	0	-5.961096	-4.179826	-2.124571

3cU+NH_4^+

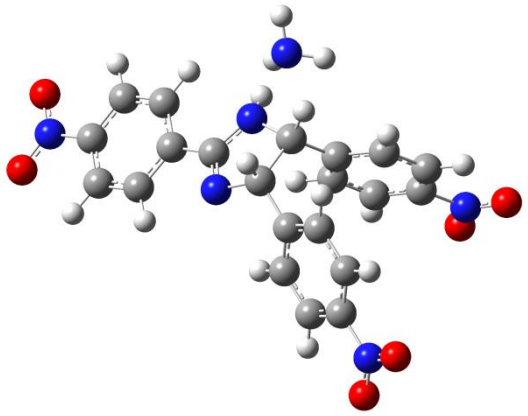


Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-4176158.313	kJ·mol^{-1}
Enthalpy (H)	-4175080.813	kJ·mol^{-1}
Gibbs free energy (G)	-4175339.731	kJ·mol^{-1}
ZPVE	995.158	kJ·mol^{-1}
Correction to U	1075.021	kJ·mol^{-1}
Correction to H	1077.500	kJ·mol^{-1}
Correction to G	818.581	kJ·mol^{-1}
S_{total}	868.439	J·mol^{-1}·K^{-1}
S_{vib}	522.464	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.490516	-1.113988	-0.202639
2	6	0	-1.597814	-0.981697	-0.521573
3	6	0	0.002411	0.777417	-0.229368
4	1	0	0.731399	-1.894834	-0.152616
5	1	0	-0.916771	-1.692359	-0.990179
6	7	0	-1.253803	0.228546	-0.185964
7	7	0	1.218921	0.162471	-0.261688
8	6	0	-2.967017	-1.447044	-0.366162
9	6	0	-3.311351	-2.744146	-0.808698
10	6	0	-3.973591	-0.650811	0.228911
11	6	0	-4.601533	-3.231294	-0.672317
12	1	0	-2.550521	-3.369418	-1.266798
13	6	0	-5.265538	-1.124411	0.369533
14	1	0	-3.714791	0.343604	0.573519
15	6	0	-5.572238	-2.416091	-0.080591
16	1	0	-4.870394	-4.223180	-1.012021
17	1	0	-6.042577	-0.520031	0.819990
18	6	0	2.860725	-1.587612	-0.147014
19	6	0	3.108876	-2.974399	-0.012615
20	6	0	3.973350	-0.715295	-0.232932
21	6	0	4.399326	-3.473268	0.045646
22	1	0	2.268897	-3.660596	0.047904
23	6	0	5.266356	-1.201138	-0.176774
24	1	0	3.794252	0.347082	-0.349055
25	6	0	5.475069	-2.581064	-0.034884
26	1	0	4.591533	-4.533205	0.151765
27	1	0	6.120634	-0.539157	-0.241366
28	6	0	0.038218	2.248226	-0.229138
29	6	0	1.267253	2.957303	-0.264909
30	6	0	-1.155857	3.015061	-0.195308
31	6	0	1.305604	4.339287	-0.258480
32	1	0	2.189636	2.392310	-0.302545
33	6	0	-1.127283	4.397871	-0.178820
34	1	0	-2.106097	2.496598	-0.192051
35	6	0	0.105880	5.063188	-0.208522
36	1	0	2.247176	4.873025	-0.289654
37	1	0	-2.042588	4.975786	-0.151949
38	1	0	0.052816	0.895553	1.877186
39	1	0	0.909905	1.264008	3.281350
40	1	0	-0.756977	1.206757	3.322841
41	1	0	0.122498	-0.201397	3.151782
42	7	0	0.081911	0.791433	2.911852
43	7	0	0.141358	6.503774	-0.191620
44	8	0	-0.933326	7.123929	-0.146879
45	8	0	1.245815	7.070361	-0.217778
46	7	0	6.827346	-3.092424	0.029369
47	8	0	7.766593	-2.286888	-0.042163
48	8	0	6.990843	-4.314592	0.155907
49	7	0	-6.924086	-2.918906	0.072796
50	8	0	-7.767112	-2.185604	0.606807
51	8	0	-7.177527	-4.059877	-0.336067

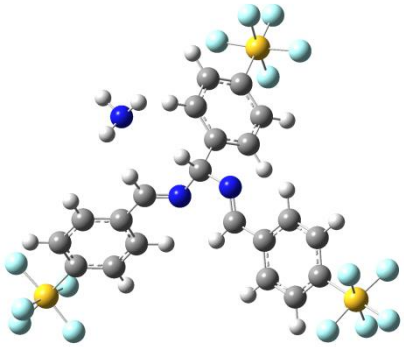
3+NH_3

Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-4176285.290	kJ·mol^{-1}
Enthalpy (H)	-4175203.602	kJ·mol^{-1}
Gibbs free energy (G)	-4175459.362	kJ·mol^{-1}
ZPVE	1001.751	kJ·mol^{-1}
Correction to U	1079.209	kJ·mol^{-1}
Correction to H	1081.687	kJ·mol^{-1}
Correction to G	825.928	kJ·mol^{-1}
S_{total}	857.846	J·mol^{-1}·K^{-1}
S_{vib}	515.665	J·mol^{-1}·K^{-1}



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-0.255422	-1.196643	-1.627729
2	6	0	-0.164027	0.372004	-1.914223
3	6	0	1.756948	-0.510402	-1.012505
4	1	0	-0.188303	-1.688208	-2.609199
5	1	0	-0.444812	0.556435	-2.954996
6	7	0	1.273466	0.567947	-1.717557
7	1	0	1.639336	1.528048	-1.593729
8	7	0	0.962050	-1.524975	-0.881228
9	6	0	-1.024322	1.263790	-1.032469
10	6	0	-2.254575	1.732169	-1.517992
11	6	0	-0.628190	1.623976	0.264854
12	6	0	-3.079522	2.532713	-0.735124
13	1	0	-2.569066	1.472835	-2.524410
14	6	0	-1.438075	2.424423	1.063490
15	1	0	0.325340	1.284562	0.653483
16	6	0	-2.656639	2.868019	0.550341
17	1	0	-4.027856	2.901021	-1.104476
18	1	0	-1.141792	2.706056	2.065680
19	6	0	-1.528035	-1.681619	-0.967347
20	6	0	-2.682064	-1.881072	-1.740581
21	6	0	-1.577685	-1.939441	0.408982
22	6	0	-3.867697	-2.314498	-1.158677
23	1	0	-2.650636	-1.701656	-2.811260
24	6	0	-2.753149	-2.379192	1.009581
25	1	0	-0.679856	-1.807552	1.001405
26	6	0	-3.885267	-2.557593	0.215108
27	1	0	-4.763166	-2.472262	-1.745618
28	1	0	-2.803152	-2.585251	2.071047
29	6	0	3.135692	-0.518982	-0.470116
30	6	0	3.507444	-1.533530	0.428014
31	6	0	4.078232	0.450825	-0.845942
32	6	0	4.791217	-1.576781	0.954042
33	1	0	2.774221	-2.282292	0.702159
34	6	0	5.369025	0.418253	-0.327447
35	1	0	3.809662	1.229783	-1.549469
36	6	0	5.705320	-0.595034	0.567718
37	1	0	5.091598	-2.349255	1.649872
38	1	0	6.108819	1.156435	-0.608243
39	1	0	2.737937	3.642843	-0.695882
40	1	0	2.578895	3.771576	-2.309579
41	1	0	1.274805	3.914897	-1.348471
42	7	0	2.136511	3.387806	-1.476669
43	7	0	7.063545	-0.631713	1.119949
44	8	0	7.856354	0.244917	0.769055
45	8	0	7.344073	-1.537012	1.908047
46	7	0	-3.512327	3.716820	1.382717
47	8	0	-4.583455	4.103411	0.909496
48	8	0	-3.119274	4.003744	2.515976
49	7	0	-5.126653	-3.020838	0.837870
50	8	0	-6.117488	-3.171360	0.118317
51	8	0	-5.123132	-3.237656	2.052141

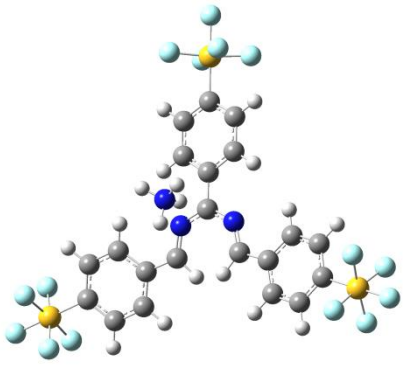
5hb+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-9627970.211	kJ·mol^{-1}
Enthalpy (H)	-9626834.686	kJ·mol^{-1}
Gibbs free energy (G)	-9627157.298	kJ·mol^{-1}
ZPVE	1026.471	kJ·mol^{-1}
Correction to U	1133.046	kJ·mol^{-1}
Correction to H	1135.524	kJ·mol^{-1}
Correction to G	812.913	kJ·mol^{-1}
S_{total}	1082.070	J·mol^{-1}·K^{-1}
S_{vib}	721.150	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.713427	-0.651068	0.587245
2	6	0	-1.886061	-0.428099	1.465956
3	6	0	0.070071	0.858215	1.381333
4	1	0	0.928745	-1.321257	0.221699
5	1	0	-1.986615	-0.141519	2.522108
6	7	0	-0.913436	-0.020917	0.744344
7	7	0	1.453761	0.456379	1.165946
8	6	0	-2.946147	-1.300894	0.926331
9	6	0	-3.946258	-1.774781	1.786116
10	6	0	-2.974283	-1.669515	-0.428180
11	6	0	-4.957750	-2.609510	1.314728
12	1	0	-3.936060	-1.492017	2.834464
13	6	0	-3.976462	-2.499064	-0.915764
14	1	0	-2.203226	-1.294951	-1.091707
15	6	0	-4.955377	-2.959643	-0.032753
16	1	0	-5.724147	-2.972361	1.986910
17	1	0	-3.993881	-2.779120	-1.960878
18	6	0	3.101666	-1.102739	0.368562
19	6	0	3.326769	-2.329369	-0.270454
20	6	0	4.200904	-0.334326	0.783732
21	6	0	4.621914	-2.791396	-0.496436
22	1	0	2.483402	-2.931001	-0.596242
23	6	0	5.499297	-0.779352	0.566810
24	1	0	4.022713	0.614454	1.277032
25	6	0	5.690447	-2.006088	-0.072529
26	1	0	4.785544	-3.739709	-0.991101
27	1	0	6.342318	-0.182416	0.889464
28	6	0	-0.145129	2.273726	0.846765
29	6	0	-0.943275	3.167131	1.568178
30	6	0	0.404971	2.675250	-0.374431
31	6	0	-1.191924	4.450376	1.083388
32	1	0	-1.370403	2.855205	2.517295
33	6	0	0.167755	3.953478	-0.875612
34	1	0	1.031790	1.991552	-0.936309
35	6	0	-0.630901	4.823780	-0.135918
36	1	0	-1.806707	5.137881	1.649724
37	1	0	0.599096	4.257471	-1.820468
38	1	0	-0.076091	0.890663	2.471558
39	1	0	-1.551272	0.457166	5.209063
40	1	0	-0.749272	1.861364	5.092491
41	1	0	-2.371347	1.849999	5.067241
42	7	0	-1.551206	1.352892	4.724752
43	16	0	-0.947452	6.497278	-0.781496
44	9	0	-2.544161	6.407749	-0.450448
45	9	0	-1.228915	5.946178	-2.292614
46	9	0	-1.231728	7.994471	-1.360022
47	9	0	0.621859	6.731603	-1.167558
48	9	0	-0.693429	7.193746	0.673766
49	16	0	7.389940	-2.598319	-0.360463
50	9	0	7.034229	-4.104935	0.157231
51	9	0	7.867174	-2.193074	1.146995
52	9	0	8.908698	-3.126895	-0.616732
53	9	0	7.886480	-1.141279	-0.902621
54	9	0	7.054176	-3.053675	-1.891564
55	16	0	-6.269914	-4.052826	-0.665900
56	9	0	-6.123603	-5.081919	0.592711
57	9	0	-5.211580	-4.951811	-1.523627
58	9	0	-7.442848	-5.030184	-1.231415
59	9	0	-6.523258	-3.113823	-1.976383
60	9	0	-7.436597	-3.244450	0.139579

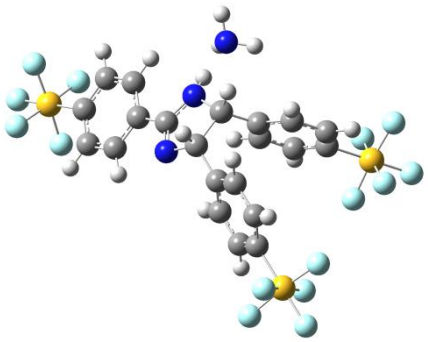
5cU+NH_4^+



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-9627908.524	kJ·mol^{-1}
Enthalpy (H)	-9626770.392	kJ·mol^{-1}
Gibbs free energy (G)	-9627087.406	kJ·mol^{-1}
ZPVE	1028.828	kJ·mol^{-1}
Correction to U	1135.654	kJ·mol^{-1}
Correction to H	1138.132	kJ·mol^{-1}
Correction to G	821.119	kJ·mol^{-1}
S_{total}	1063.297	J·mol^{-1}·K^{-1}
S_{vib}	702.008	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.534331	-1.235037	-0.174311
2	6	0	-1.589889	-1.165550	-0.402811
3	6	0	-0.002562	0.625439	-0.149272
4	1	0	0.803877	-2.042923	-0.146031
5	1	0	-0.895716	-1.923797	-0.763594
6	7	0	-1.252905	0.064580	-0.141137
7	7	0	1.226236	0.031481	-0.195514
8	6	0	-2.978331	-1.602184	-0.301804
9	6	0	-3.320148	-2.921768	-0.662150
10	6	0	-4.008202	-0.752700	0.156474
11	6	0	-4.629371	-3.381078	-0.578585
12	1	0	-2.546083	-3.596008	-1.017758
13	6	0	-5.320055	-1.194981	0.244637
14	1	0	-3.759090	0.263235	0.440791
15	6	0	-5.620081	-2.510172	-0.123830
16	1	0	-4.868986	-4.397527	-0.863363
17	1	0	-6.096569	-0.526974	0.595274
18	6	0	2.925002	-1.670412	-0.137760
19	6	0	3.219366	-3.047488	-0.049921
20	6	0	4.007955	-0.766027	-0.196601
21	6	0	4.529236	-3.510100	-0.013634
22	1	0	2.405197	-3.765823	-0.008671
23	6	0	5.321028	-1.211489	-0.162314
24	1	0	3.799425	0.294536	-0.276549
25	6	0	5.571876	-2.584270	-0.068681
26	1	0	4.730368	-4.571460	0.055664
27	1	0	6.136763	-0.501177	-0.210221
28	6	0	0.013628	2.104155	-0.155276
29	6	0	1.227642	2.830012	-0.144782
30	6	0	-1.184643	2.855870	-0.163989
31	6	0	1.250520	4.217807	-0.133714
32	1	0	2.161132	2.281793	-0.149046
33	6	0	-1.177442	4.244266	-0.145292
34	1	0	-2.129909	2.329127	-0.196016
35	6	0	0.043722	4.921334	-0.127366
36	1	0	2.198492	4.741278	-0.128507
37	1	0	-2.113904	4.788007	-0.153236
38	1	0	0.017744	0.637521	1.847374
39	1	0	0.850171	1.010245	3.273925
40	1	0	-0.816922	1.015844	3.269038
41	1	0	0.012148	-0.427032	3.163272
42	7	0	0.016184	0.558425	2.893533
43	16	0	0.063230	6.729200	-0.102099
44	9	0	1.217394	6.788429	1.058158
45	9	0	-1.097952	6.813838	1.049566
46	9	0	0.081068	8.364129	-0.073936
47	9	0	-1.089314	6.851116	-1.256175
48	9	0	1.226709	6.825866	-1.247626
49	16	0	7.285225	-3.173917	-0.022459
50	9	0	6.984515	-4.214024	1.203835
51	9	0	7.738565	-2.032091	1.057277
52	9	0	8.829304	-3.704277	0.020641
53	9	0	7.747607	-2.189540	-1.242519
54	9	0	6.994459	-4.372475	-1.095334
55	16		-7.331340	-3.097916	-0.003145
56	9		-7.280116	-3.814813	-1.470691
57	9		-7.935511	-1.740946	-0.684544
58	9		-8.871942	-3.626417	0.107795
59	9		-7.542740	-2.436163	1.477666
60	9		-6.887610	-4.510620	0.691289

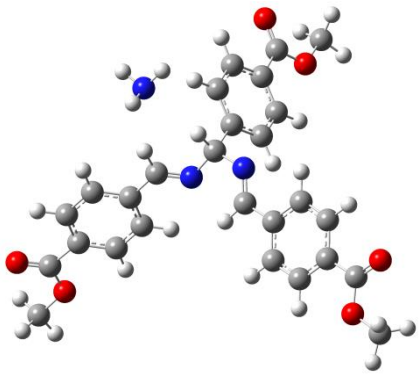
5hb+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-9628058.448	kJ·mol^{-1}
Enthalpy (H)	-9626914.547	kJ·mol^{-1}
Gibbs free energy (G)	-9627224.847	kJ·mol^{-1}
ZPVE	1037.489	kJ·mol^{-1}
Correction to U	1141.420	kJ·mol^{-1}
Correction to H	1143.901	kJ·mol^{-1}
Correction to G	833.600	kJ·mol^{-1}
S_{total}	1040.770	J·mol^{-1}·K^{-1}
S_{vib}	683.716	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000331	-1.378629	2.036232
2	6	0	-0.075760	0.165446	2.431532
3	6	0	-1.996549	-0.623569	1.449540
4	1	0	-0.089592	-1.938562	2.978459
5	1	0	0.201050	0.274368	3.483914
6	7	0	-1.510306	0.390977	2.242919
7	1	0	-1.862645	1.361538	2.183020
8	7	0	-1.211701	-1.634338	1.249225
9	6	0	0.799059	1.106456	1.616876
10	6	0	2.039056	1.511377	2.126686
11	6	0	0.410040	1.571119	0.353786
12	6	0	2.882228	2.349446	1.399938
13	1	0	2.355310	1.172153	3.108705
14	6	0	1.236431	2.411076	-0.389948
15	1	0	-0.551037	1.284194	-0.058263
16	6	0	2.466280	2.788069	0.145090
17	1	0	3.835784	2.653010	1.812247
18	1	0	0.922070	2.759435	-1.365175
19	6	0	1.274598	-1.832987	1.358291
20	6	0	2.394400	-2.173273	2.127498
21	6	0	1.362956	-1.918076	-0.035403
22	6	0	3.585124	-2.577596	1.527867
23	1	0	2.340127	-2.130998	3.211712
24	6	0	2.542617	-2.323801	-0.656510
25	1	0	0.493030	-1.678130	-0.635992
26	6	0	3.641138	-2.645451	0.137398
27	1	0	4.441424	-2.839327	2.135654
28	1	0	2.597017	-2.387276	-1.735601
29	6	0	-3.367859	-0.568190	0.890831
30	6	0	-3.740564	-1.493343	-0.095271
31	6	0	-4.304075	0.376009	1.333048
32	6	0	-5.017816	-1.472725	-0.643983
33	1	0	-3.015920	-2.228155	-0.425334
34	6	0	-5.589567	0.407172	0.795110
35	1	0	-4.040763	1.089888	2.104699
36	6	0	-5.926720	-0.517106	-0.189576
37	1	0	-5.293369	-2.187681	-1.408117
38	1	0	-6.306797	1.137952	1.144932
39	1	0	-2.941000	3.559226	1.447778
40	1	0	-2.747123	3.574404	3.062753
41	1	0	-1.459340	3.754687	2.085786
42	7	0	-2.330233	3.238881	2.196546
43	16	0	3.553830	3.884825	-0.818818
44	9	0	2.324263	4.884319	-1.216316
45	9	0	3.306659	3.046196	-2.197117
46	9	0	4.526838	4.866380	-1.682067
47	9	0	4.874830	2.980827	-0.502608
48	9	0	3.891655	4.819102	0.477682
49	16	0	5.187678	-3.177284	-0.661960
50	9	0	5.390094	-4.422447	0.376078
51	9	0	6.104129	-2.232958	0.305561
52	9	0	6.573606	-3.652225	-1.376860
53	9	0	5.119970	-1.979101	-1.769348
54	9	0	4.406489	-4.168740	-1.698292
55	16		-7.602525	-0.478159	-0.904735
56	9		-7.762010	-2.099490	-0.814140
57	9		-7.036810	-0.625906	-2.428570
58	9		-9.099490	-0.442015	-1.545131
59	9		-7.582498	1.147631	-1.055112
60	9		-8.307102	-0.325800	0.559799

7hb+NH_3

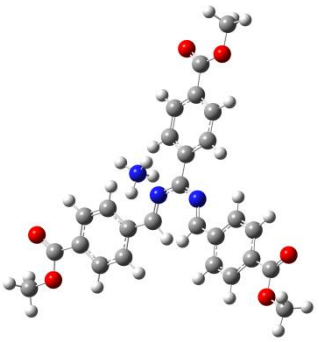


Thermodynamic quantities at 298.15K and 1.00 atm

Electronic Energy (E)	-4360359.851	$kJ \cdot mol^{-1}$
Enthalpy (H)	-4358950.494	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-4359264.796	$kJ \cdot mol^{-1}$
ZPVE	1307.873	$kJ \cdot mol^{-1}$
Correction to U	1406.878	$kJ \cdot mol^{-1}$
Correction to H	1409.357	$kJ \cdot mol^{-1}$
Correction to G	1095.055	$kJ \cdot mol^{-1}$
S_{total}	1054.196	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	704.176	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.709694	-0.586479	0.486711
2	6	0	-1.905064	-0.416733	1.329525
3	6	0	0.027525	0.902449	1.244856
4	1	0	0.939699	-1.268900	0.111330
5	1	0	-2.012096	-0.119026	2.382443
6	7	0	-0.933620	-0.001839	0.609179
7	7	0	1.422006	0.519317	1.057260
8	6	0	-2.952283	-1.310146	0.802284
9	6	0	-3.960433	-1.766016	1.666078
10	6	0	-2.966650	-1.717523	-0.543080
11	6	0	-4.959544	-2.613975	1.199869
12	1	0	-3.957249	-1.452402	2.706265
13	6	0	-3.963523	-2.562398	-1.011825
14	1	0	-2.187974	-1.357129	-1.206108
15	6	0	-4.968285	-3.017774	-0.141193
16	1	0	-5.741473	-2.971845	1.860164
17	1	0	-3.972926	-2.873616	-2.049694
18	6	0	3.106139	-1.020970	0.292661
19	6	0	3.357213	-2.257329	-0.321416
20	6	0	4.192140	-0.229446	0.706263
21	6	0	4.661734	-2.701169	-0.520623
22	1	0	2.522399	-2.873509	-0.643922
23	6	0	5.493122	-0.668284	0.508872
24	1	0	3.991697	0.725788	1.178735
25	6	0	5.739255	-1.907388	-0.105598
26	1	0	4.848054	-3.657166	-0.995148
27	1	0	6.337958	-0.065352	0.823045
28	6	0	-0.196262	2.306122	0.684174
29	6	0	-0.900506	3.251856	1.438695
30	6	0	0.260115	2.649681	-0.594469
31	6	0	-1.139446	4.523698	0.925638
32	1	0	-1.258741	2.982620	2.428520
33	6	0	0.022544	3.919377	-1.112119
34	1	0	0.810587	1.921384	-1.181039
35	6	0	-0.679982	4.867382	-0.352696
36	1	0	-1.679511	5.265055	1.504501
37	1	0	0.380216	4.181638	-2.100924
38	1	0	-0.134992	0.949648	2.332476
39	1	0	-1.283814	0.429131	5.136222
40	1	0	-0.787384	1.966993	5.004510
41	1	0	-2.373430	1.629123	5.053486
42	7	0	-1.487442	1.309358	4.666700
43	6	0	7.156934	-2.327743	-0.291800
44	8	0	8.120431	-1.665582	0.053552
45	8	0	7.266140	-3.531244	-0.889163
46	6	0	8.609274	-4.003465	-1.103903
47	1	0	9.134847	-4.107741	-0.152195
48	1	0	8.504454	-4.972224	-1.590132
49	1	0	9.160209	-3.311266	-1.744322
50	6	0	-0.958906	6.241720	-0.853376
51	8	0	-1.568358	7.093151	-0.228251
52	8	0	-0.460960	6.454405	-2.089018
53	6	0	-0.691102	7.764329	-2.639063
54	1	0	-0.234401	8.530425	-2.008523
55	1	0	-0.226046	7.754176	-3.623805
56	1	0	-1.762006	7.961731	-2.723996
57	6	0	-6.062029	-3.925665	-0.591295
58	8	0	-6.943150	-4.351476	0.135438
59	8	0	-5.974562	-4.230036	-1.900925
60	6	0	-6.999542	-5.103813	-2.410552
61	1	0	-7.986207	-4.655952	-2.274138
62	1	0	-6.778757	-5.226771	-3.469756
63	1	0	-6.968859	-6.068206	-1.898722

7cU+NH_4^+

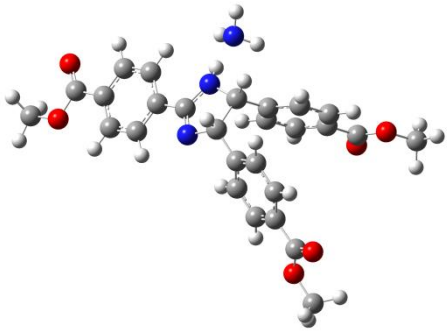


Thermodynamic quantities at 298.15K and 1.00 atm

Electronic Energy (E)	-4360291.676	kJ·mol^{-1}
Enthalpy (H)	-4358882.094	kJ·mol^{-1}
Gibbs free energy (G)	-4359178.372	kJ·mol^{-1}
ZPVE	1310.955	kJ·mol^{-1}
Correction to U	1407.104	kJ·mol^{-1}
Correction to H	1409.582	kJ·mol^{-1}
Correction to G	1113.304	kJ·mol^{-1}
S_{total}	993.746	J·mol^{-1}·K^{-1}
S_{vib}	643.462	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.410957	-1.168461	-0.234089
2	6	0	-1.693830	-0.894094	-0.461084
3	6	0	0.001562	0.791888	-0.210077
4	1	0	0.624582	-1.923418	-0.216169
5	1	0	-1.051445	-1.667184	-0.882503
6	7	0	-1.281550	0.307327	-0.172132
7	7	0	1.188033	0.117780	-0.259637
8	6	0	-3.094103	-1.270866	-0.313332
9	6	0	-3.510410	-2.562928	-0.701170
10	6	0	-4.066067	-0.393325	0.218917
11	6	0	-4.833504	-2.963102	-0.571959
12	1	0	-2.778579	-3.253729	-1.112164
13	6	0	-5.385969	-0.790895	0.347428
14	1	0	-3.756858	0.600461	0.523428
15	6	0	-5.790903	-2.080820	-0.043831
16	1	0	-5.133607	-3.958625	-0.878276
17	1	0	-6.131214	-0.114569	0.752978
18	6	0	2.765272	-1.698981	-0.177080
19	6	0	2.961152	-3.096210	-0.097222
20	6	0	3.913213	-0.872778	-0.205542
21	6	0	4.234391	-3.645653	-0.041731
22	1	0	2.093675	-3.751321	-0.078703
23	6	0	5.183312	-1.419993	-0.151216
24	1	0	3.778530	0.200900	-0.274799
25	6	0	5.366642	-2.813395	-0.067079
26	1	0	4.360888	-4.720566	0.020070
27	1	0	6.061521	-0.783108	-0.173621
28	6	0	0.109029	2.265928	-0.210587
29	6	0	1.366146	2.918251	-0.244331
30	6	0	-1.042173	3.091516	-0.169081
31	6	0	1.467443	4.300728	-0.228202
32	1	0	2.261841	2.310959	-0.289025
33	6	0	-0.938621	4.472885	-0.143624
34	1	0	-2.017520	2.620550	-0.165996
35	6	0	0.315886	5.107270	-0.170945
36	1	0	2.445541	4.768369	-0.259066
37	1	0	-1.831909	5.088505	-0.110464
38	1	0	0.056047	0.826220	1.775236
39	1	0	0.885442	1.195320	3.205116
40	1	0	-0.781979	1.188713	3.198604
41	1	0	0.058283	-0.247381	3.082595
42	7	0	0.054994	0.740204	2.821344
43	6	0	0.365946	6.581880	-0.144168
44	8	0	-0.610824	7.316082	-0.089550
45	8	0	1.632981	7.065865	-0.183014
46	6	0	1.751716	8.497029	-0.163597
47	1	0	1.314831	8.910051	0.748937
48	1	0	2.820817	8.704405	-0.199391
49	1	0	1.250209	8.938971	-1.027943
50	6	0	6.748580	-3.339025	-0.011337
51	8	0	7.757489	-2.649937	-0.036750
52	8	0	6.792391	-4.689810	0.074538
53	6	0	8.107378	-5.267287	0.130687
54	1	0	8.651341	-4.904555	1.006046
55	1	0	7.953049	-6.343590	0.198577
56	1	0	8.676020	-5.020452	-0.768940
57	6	0	-7.215434	-2.451253	0.120532
58	8	0	-8.075091	-1.718901	0.586505
59	8	0	-7.481547	-3.708189	-0.304579
60	6	0	-8.849521	-4.131387	-0.177138
61	1	0	-9.508665	-3.485362	-0.761679
62	1	0	-8.878647	-5.150554	-0.560708
63	1	0	-9.164274	-4.108589	0.868798

7+NH_3

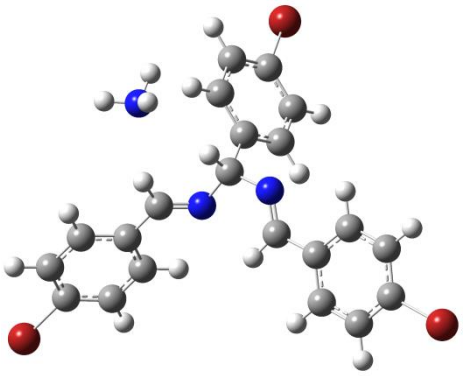


Thermodynamic quantities at 298.15K and 1.00 atm

Electronic Energy (E)	-4360446.305	$kJ \cdot mol^{-1}$
Enthalpy (H)	-4359031.132	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-4359323.235	$kJ \cdot mol^{-1}$
ZPVE	1318.877	$kJ \cdot mol^{-1}$
Correction to U	1412.695	$kJ \cdot mol^{-1}$
Correction to H	1415.173	$kJ \cdot mol^{-1}$
Correction to G	1123.070	$kJ \cdot mol^{-1}$
S_{total}	979.746	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	633.361	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-0.083601	-1.133375	-1.932688
2	6	0	-0.053786	0.446034	-2.155717
3	6	0	1.897627	-0.391807	-1.276074
4	1	0	0.015440	-1.581644	-2.932649
5	1	0	-0.344976	0.659903	-3.188384
6	7	0	1.377727	0.688764	-1.956978
7	1	0	1.695808	1.654064	-1.771682
8	7	0	1.141523	-1.439985	-1.185619
9	6	0	-0.944998	1.270471	-1.239729
10	6	0	-2.202593	1.689650	-1.696007
11	6	0	-0.555708	1.618892	0.062294
12	6	0	-3.055381	2.428100	-0.880383
13	1	0	-2.516507	1.436979	-2.705051
14	6	0	-1.400947	2.359458	0.882389
15	1	0	0.417823	1.317302	0.433890
16	6	0	-2.658619	2.770174	0.419822
17	1	0	-4.023442	2.745944	-1.249539
18	1	0	-1.100756	2.628598	1.889270
19	6	0	-1.342361	-1.695939	-1.308109
20	6	0	-2.461986	-1.964326	-2.109159
21	6	0	-1.419741	-1.953930	0.066021
22	6	0	-3.633506	-2.463393	-1.550784
23	1	0	-2.411325	-1.786140	-3.180207
24	6	0	-2.587429	-2.459481	0.631614
25	1	0	-0.548235	-1.767909	0.683877
26	6	0	-3.706619	-2.715341	-0.173547
27	1	0	-4.500279	-2.672139	-2.168314
28	1	0	-2.634970	-2.659243	1.695848
29	6	0	3.269471	-0.353898	-0.718206
30	6	0	3.671528	-1.353007	0.182965
31	6	0	4.182319	0.649319	-1.078988
32	6	0	4.951659	-1.344990	0.722549
33	1	0	2.963343	-2.129109	0.449015
34	6	0	5.465082	0.657183	-0.540311
35	1	0	3.893787	1.418460	-1.786210
36	6	0	5.859385	-0.335711	0.365083
37	1	0	5.253240	-2.116304	1.421196
38	1	0	6.177314	1.427034	-0.815561
39	1	0	2.861521	3.777037	-0.892077
40	1	0	2.242167	4.078444	-2.366094
41	1	0	1.254733	3.943114	-1.079030
42	7	0	2.087185	3.547445	-1.511476
43	6	0	7.243661	-0.274936	0.914086
44	8	0	8.056409	0.589866	0.634809
45	8	0	7.507497	-1.287899	1.762837
46	6	0	-3.520884	3.562689	1.338534
47	8	0	-3.207334	3.882781	2.472795
48	8	0	-4.702963	3.897008	0.781406
49	6	0	-4.979718	-3.256604	0.374129
50	8	0	-5.973115	-3.493194	-0.293115
51	8	0	-4.925754	-3.463551	1.706654
52	6	0	8.828414	-1.297983	2.335633
53	1	0	8.861212	-2.175619	2.979451
54	1	0	9.584885	-1.369982	1.551205
55	1	0	8.999829	-0.389868	2.917746
56	6	0	-5.592362	4.662264	1.614953
57	1	0	-6.476372	4.848126	1.006643
58	1	0	-5.857464	4.097509	2.511519
59	1	0	-5.125392	5.604517	1.909803
60	6	0	-6.123710	-3.988144	2.306598
61	1	0	-6.378054	-4.957093	1.871289
62	1	0	-5.898196	-4.094037	3.366843
63	1	0	-6.959263	-3.299799	2.160804

8hb+NH_3

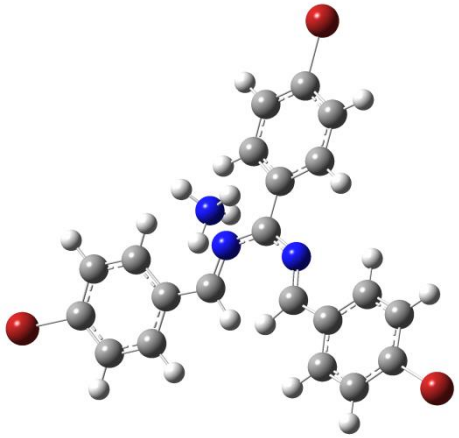


Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-22816289.583	kJ·mol^{-1}
Enthalpy (H)	-22815321.317	kJ·mol^{-1}
Gibbs free energy (G)	-22815584.525	kJ·mol^{-1}
ZPVE	891.514	kJ·mol^{-1}
Correction to U	965.788	kJ·mol^{-1}
Correction to H	968.266	kJ·mol^{-1}
Correction to G	705.058	kJ·mol^{-1}
S_{total}	882.820	J·mol^{-1}·K^{-1}
S_{vib}	530.071	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.712837	-0.655270	0.380741
2	6	0	-1.897903	-0.415687	1.203825
3	6	0	0.060908	0.866780	1.139234
4	1	0	0.928468	-1.306607	-0.019485
5	1	0	-2.007494	-0.120675	2.257593
6	7	0	-0.914285	-0.014366	0.492806
7	7	0	1.447745	0.447495	0.968061
8	6	0	-2.957445	-1.287215	0.668353
9	6	0	-3.976807	-1.733198	1.521948
10	6	0	-2.973077	-1.687905	-0.678388
11	6	0	-4.991720	-2.566206	1.052903
12	1	0	-3.977629	-1.427613	2.564615
13	6	0	-3.979043	-2.516873	-1.161080
14	1	0	-2.187531	-1.337440	-1.338919
15	6	0	-4.979243	-2.948671	-0.286334
16	1	0	-5.776640	-2.910503	1.716033
17	1	0	-3.991544	-2.824688	-2.200303
18	6	0	3.096391	-1.130341	0.198850
19	6	0	3.319944	-2.354865	-0.446570
20	6	0	4.200427	-0.390936	0.655387
21	6	0	4.612968	-2.841350	-0.635854
22	1	0	2.474479	-2.935591	-0.805352
23	6	0	5.495792	-0.862536	0.474336
24	1	0	4.026260	0.556971	1.152975
25	6	0	5.687107	-2.086925	-0.170616
26	1	0	4.781160	-3.788386	-1.135086
27	1	0	6.347154	-0.291444	0.826730
28	6	0	-0.121498	2.277468	0.581940
29	6	0	-0.849268	3.223697	1.310607
30	6	0	0.391893	2.629135	-0.671191
31	6	0	-1.061749	4.506955	0.803108
32	1	0	-1.252734	2.953030	2.282924
33	6	0	0.188030	3.905934	-1.193406
34	1	0	0.963535	1.904817	-1.242356
35	6	0	-0.538881	4.831012	-0.446171
36	1	0	-1.622599	5.240549	1.371153
37	1	0	0.588987	4.177321	-2.163302
38	1	0	-0.113364	0.915620	2.225120
39	1	0	-0.882004	0.759927	4.982955
40	1	0	-1.277423	2.329524	4.897052
41	1	0	-2.442939	1.203888	4.978214
42	7	0	-1.539981	1.407556	4.553811
43	35	0	-0.821895	6.591290	-1.156176
44	35	0	7.468364	-2.744339	-0.419469
45	35	0	-6.365625	-4.091566	-0.946156

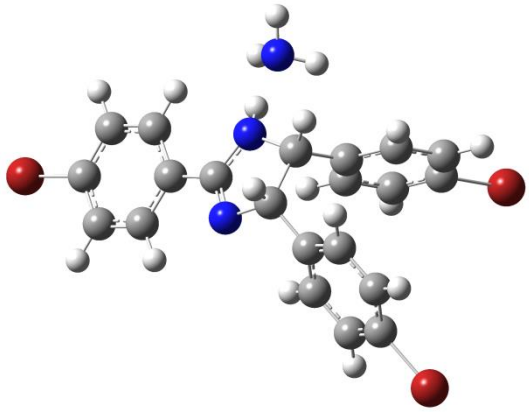
8cU+NH_4^+

Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-22816201.783	kJ·mol^{-1}
Enthalpy (H)	-22815233.593	kJ·mol^{-1}
Gibbs free energy (G)	-22815478.323	kJ·mol^{-1}
ZPVE	894.155	kJ·mol^{-1}
Correction to U	965.711	kJ·mol^{-1}
Correction to H	968.189	kJ·mol^{-1}
Correction to G	723.459	kJ·mol^{-1}
S_{total}	820.851	J·mol^{-1}·K^{-1}
S_{vib}	467.855	J·mol^{-1}·K^{-1}



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.534492	-1.165106	-0.167094
2	6	0	-1.594088	-1.101166	-0.375185
3	6	0	-0.006429	0.696925	-0.144451
4	1	0	0.804702	-1.973874	-0.132730
5	1	0	-0.896940	-1.867859	-0.713010
6	7	0	-1.257204	0.134324	-0.137863
7	7	0	1.222828	0.101352	-0.196530
8	6	0	-2.984288	-1.539867	-0.277042
9	6	0	-3.322096	-2.866967	-0.611290
10	6	0	-4.022070	-0.685653	0.153009
11	6	0	-4.633824	-3.327814	-0.529678
12	1	0	-2.542595	-3.547180	-0.945342
13	6	0	-5.335630	-1.131727	0.238150
14	1	0	-3.777633	0.337173	0.418556
15	6	0	-5.632023	-2.453165	-0.104258
16	1	0	-4.876337	-4.351278	-0.793385
17	1	0	-6.124282	-0.463705	0.567237
18	6	0	2.927022	-1.603112	-0.133878
19	6	0	3.222395	-2.979602	-0.047542
20	6	0	4.012756	-0.702678	-0.195248
21	6	0	4.534781	-3.444423	-0.016614
22	1	0	2.406874	-3.697423	-0.004079
23	6	0	5.327299	-1.152687	-0.166026
24	1	0	3.805776	0.358993	-0.273694
25	6	0	5.579413	-2.523682	-0.075244
26	1	0	4.742161	-4.506740	0.050862
27	1	0	6.151328	-0.449031	-0.216057
28	6	0	0.009567	2.181035	-0.162697
29	6	0	1.221006	2.908329	-0.143793
30	6	0	-1.186247	2.933599	-0.186737
31	6	0	1.242456	4.300122	-0.139776
32	1	0	2.155297	2.360112	-0.135637
33	6	0	-1.178172	4.325948	-0.175836
34	1	0	-2.131571	2.405865	-0.222120
35	6	0	0.039177	5.003779	-0.150438
36	1	0	2.188080	4.831958	-0.128094
37	1	0	-2.112213	4.877636	-0.195615
38	1	0	0.080557	0.659498	1.779277
39	1	0	0.988982	0.921681	3.192122
40	1	0	-0.675099	0.892318	3.284443
41	1	0	0.168443	-0.515968	2.996880
42	7	0	0.141122	0.489673	2.820903
43	35	0	7.394205	-3.148158	-0.035666
44	35	0	-7.443663	-3.075110	0.017761
45	35	0	0.059865	6.926636	-0.138243

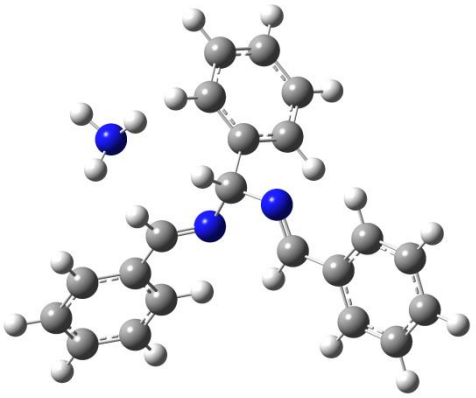
8+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-22816373.427	kJ·mol^{-1}
Enthalpy (H)	-22815399.384	kJ·mol^{-1}
Gibbs free energy (G)	-22815640.641	kJ·mol^{-1}
ZPVE	902.271	kJ·mol^{-1}
Correction to U	971.564	kJ·mol^{-1}
Correction to H	974.043	kJ·mol^{-1}
Correction to G	732.786	kJ·mol^{-1}
S_{total}	809.198	J·mol^{-1}·K^{-1}
S_{vib}	460.378	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	0.157093	-1.307338	1.760226
2	6	0	0.068496	0.243334	2.119771
3	6	0	-1.851293	-0.585695	1.163544
4	1	0	0.074942	-1.845084	2.716687
5	1	0	0.349626	0.376978	3.168695
6	7	0	-1.371577	0.450074	1.937846
7	1	0	-1.722115	1.415176	1.833020
8	7	0	-1.056216	-1.592948	0.984820
9	6	0	0.927297	1.180522	1.284626
10	6	0	2.153397	1.630955	1.789963
11	6	0	0.539961	1.603258	0.005834
12	6	0	2.981291	2.472179	1.046260
13	1	0	2.470603	1.325088	2.783327
14	6	0	1.352434	2.446330	-0.752988
15	1	0	-0.410380	1.280899	-0.406706
16	6	0	2.568815	2.870439	-0.222617
17	1	0	3.926271	2.815814	1.451090
18	1	0	1.042878	2.766634	-1.741385
19	6	0	1.434594	-1.768275	1.091024
20	6	0	2.558907	-2.083125	1.864581
21	6	0	1.526220	-1.885438	-0.300310
22	6	0	3.753746	-2.492269	1.271972
23	1	0	2.504679	-2.015867	2.948237
24	6	0	2.710429	-2.297907	-0.912169
25	1	0	0.654163	-1.665243	-0.906348
26	6	0	3.814034	-2.593372	-0.115841
27	1	0	4.617692	-2.735636	1.879693
28	1	0	2.771379	-2.389888	-1.990630
29	6	0	-3.223614	-0.550470	0.608735
30	6	0	-3.604474	-1.511328	-0.340758
31	6	0	-4.160813	0.408608	1.018275
32	6	0	-4.886414	-1.511920	-0.881113
33	1	0	-2.880557	-2.257362	-0.648038
34	6	0	-5.450450	0.417240	0.486606
35	1	0	-3.893407	1.151840	1.760932
36	6	0	-5.797721	-0.543133	-0.459834
37	1	0	-5.174649	-2.253213	-1.617402
38	1	0	-6.173299	1.158125	0.808091
39	1	0	-2.923146	3.613093	1.132678
40	1	0	-2.330629	3.772091	2.639446
41	1	0	-1.320584	3.760252	1.363310
42	7	0	-2.159785	3.324710	1.741056
43	35	0	3.691326	4.032365	-1.255709
44	35	0	5.448264	-3.163958	-0.946067
45	35	0	-7.565362	-0.537039	-1.197523

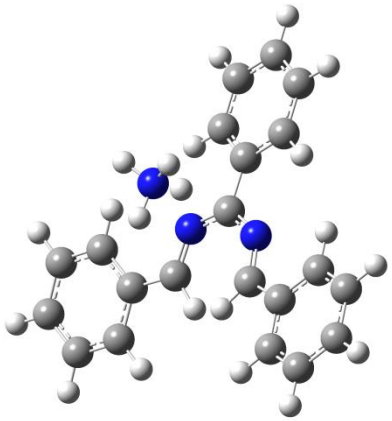
Unsubstituted hydrobenzamide+NH_3



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-2565467.569	kJ·mol^{-1}
Enthalpy (H)	-2564430.975	kJ·mol^{-1}
Gibbs free energy (G)	-2564650.478	kJ·mol^{-1}
ZPVE	971.961	kJ·mol^{-1}
Correction to U	1034.116	kJ·mol^{-1}
Correction to H	1036.594	kJ·mol^{-1}
Correction to G	817.092	kJ·mol^{-1}
S_{total}	736.238	J·mol^{-1}·K^{-1}
S_{vib}	405.626	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.783370	-0.666713	0.102811
2	6	0	-1.886939	-0.434154	0.564052
3	6	0	0.042673	0.892498	0.510810
4	1	0	1.047792	-1.381288	-0.282929
5	1	0	-2.087909	-0.024000	1.565124
6	7	0	-0.854752	-0.087189	-0.105513
7	7	0	1.446666	0.492414	0.521052
8	6	0	-2.886630	-1.388723	0.054576
9	6	0	-3.970719	-1.743530	0.871804
10	6	0	-2.782955	-1.954145	-1.228280
11	6	0	-4.932462	-2.648048	0.421088
12	1	0	-4.056545	-1.306795	1.863560
13	6	0	-3.742476	-2.855886	-1.676933
14	1	0	-1.945347	-1.670564	-1.856714
15	6	0	-4.819569	-3.205899	-0.853611
16	1	0	-5.767229	-2.915760	1.061814
17	1	0	-3.656609	-3.287909	-2.669646
18	6	0	3.183990	-1.128781	0.108068
19	6	0	3.477440	-2.420635	-0.353812
20	6	0	4.233283	-0.312034	0.563540
21	6	0	4.791039	-2.891144	-0.361264
22	1	0	2.669806	-3.056442	-0.707908
23	6	0	5.542958	-0.781567	0.555965
24	1	0	3.999204	0.686271	0.918004
25	6	0	5.826096	-2.072453	0.093677
26	1	0	5.005795	-3.892998	-0.720955
27	1	0	6.348137	-0.143929	0.909267
28	6	0	-0.110230	2.221320	-0.228226
29	6	0	-0.878196	3.245520	0.336439
30	6	0	0.473057	2.417015	-1.485866
31	6	0	-1.056998	4.452202	-0.344192
32	1	0	-1.335299	3.090420	1.310784
33	6	0	0.293384	3.621206	-2.166944
34	1	0	1.073865	1.627184	-1.926305
35	6	0	-0.471819	4.642769	-1.597418
36	1	0	-1.651441	5.242840	0.105075
37	1	0	0.751962	3.764135	-3.141383
38	1	0	-0.231747	1.066909	1.563013
39	1	0	-1.841190	0.951240	4.344446
40	1	0	-0.906898	2.251794	4.090248
41	1	0	-2.522005	2.403905	4.098949
42	7	0	-1.765822	1.798528	3.784976
43	1	0	6.849561	-2.435782	0.088822
44	1	0	-0.608924	5.581067	-2.127212
45	1	0	-5.567403	-3.909478	-1.207380

Unsubstituted carbanion+NH_4^+

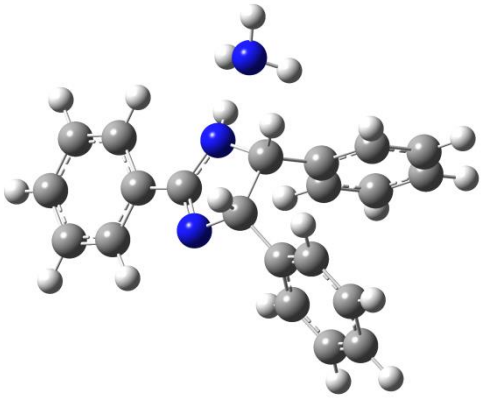


Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-2565365.846	kJ·mol^{-1}
Enthalpy (H)	-2564330.802	kJ·mol^{-1}
Gibbs free energy (G)	-2564537.340	kJ·mol^{-1}
ZPVE	973.102	kJ·mol^{-1}
Correction to U	1032.565	kJ·mol^{-1}
Correction to H	1035.044	kJ·mol^{-1}
Correction to G	828.506	kJ·mol^{-1}
S_{total}	692.749	J·mol^{-1}·K^{-1}
S_{vib}	362.464	J·mol^{-1}·K^{-1}

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	1.537474	-1.015938	-0.191826
2	6	0	-1.590929	-0.960401	-0.376501
3	6	0	-0.004301	0.847934	-0.207775
4	1	0	0.805907	-1.822577	-0.136178
5	1	0	-0.895531	-1.729807	-0.713369
6	7	0	-1.254351	0.281351	-0.172968
7	7	0	1.224874	0.249306	-0.254919
8	6	0	-2.977825	-1.406704	-0.242575
9	6	0	-3.313430	-2.739586	-0.557342
10	6	0	-4.010581	-0.554588	0.204114
11	6	0	-4.623437	-3.200525	-0.439784
12	1	0	-2.532572	-3.413758	-0.902495
13	6	0	-5.317378	-1.016811	0.319750
14	1	0	-3.761376	0.471309	0.454958
15	6	0	-5.635490	-2.342732	-0.000310
16	1	0	-4.855934	-4.231627	-0.692351
17	1	0	-6.097447	-0.342006	0.663060
18	6	0	2.930505	-1.458230	-0.144896
19	6	0	3.217574	-2.834430	-0.025354
20	6	0	4.020905	-0.564462	-0.223466
21	6	0	4.531027	-3.297869	0.019292
22	1	0	2.393600	-3.542588	0.031944
23	6	0	5.330932	-1.029901	-0.179399
24	1	0	3.814984	0.495846	-0.325857
25	6	0	5.598737	-2.399241	-0.056597
26	1	0	4.722653	-4.363651	0.112093
27	1	0	6.153859	-0.322440	-0.243822
28	6	0	0.008675	2.334060	-0.268722
29	6	0	1.218823	3.064219	-0.275546
30	6	0	-1.189549	3.082702	-0.305707
31	6	0	1.227569	4.456746	-0.312373
32	1	0	2.152663	2.514535	-0.255965
33	6	0	-1.175643	4.475789	-0.334919
34	1	0	-2.131764	2.547479	-0.319043
35	6	0	0.031521	5.180640	-0.338142
36	1	0	2.179766	4.982199	-0.320852
37	1	0	-2.119142	5.015943	-0.364358
38	1	0	0.082252	0.850090	1.677191
39	1	0	0.974485	1.120854	3.104779
40	1	0	-0.690259	1.075767	3.179504
41	1	0	0.169680	-0.323775	2.898866
42	7	0	0.134645	0.681668	2.724894
43	1	0	0.040431	6.266382	-0.367020
44	1	0	-6.656726	-2.700239	0.093000
45	1	0	6.623213	-2.758223	-0.024667

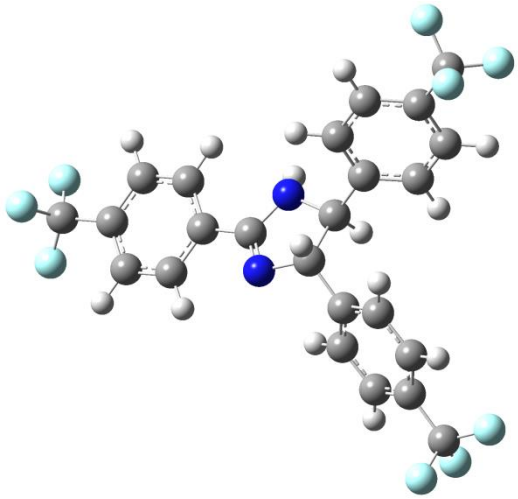
Unsubstituted amarine+NH_3

Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-2565549.101	kJ·mol^{-1}
Enthalpy (H)	-2564507.184	kJ·mol^{-1}
Gibbs free energy (G)	-2564709.175	kJ·mol^{-1}
ZPVE	982.097	kJ·mol^{-1}
Correction to U	1039.439	kJ·mol^{-1}
Correction to H	1041.918	kJ·mol^{-1}
Correction to G	839.927	kJ·mol^{-1}
S_{total}	677.498	J·mol^{-1}·K^{-1}
S_{vib}	350.657	J·mol^{-1}·K^{-1}



Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-0.620419	-1.050081	-1.203022
2	6	0	-0.440180	0.526607	-1.349733
3	6	0	1.463138	-0.548665	-0.632325
4	1	0	-0.623268	-1.449710	-2.228715
5	1	0	-0.763721	0.823390	-2.352218
6	7	0	1.020440	0.614294	-1.231423
7	1	0	1.435689	1.527003	-0.989816
8	7	0	0.608950	-1.519093	-0.549431
9	6	0	-1.182606	1.396466	-0.346543
10	6	0	-2.368067	2.036426	-0.730555
11	6	0	-0.721121	1.577475	0.965506
12	6	0	-3.080536	2.831365	0.169063
13	1	0	-2.734721	1.913836	-1.746783
14	6	0	-1.429110	2.373583	1.867290
15	1	0	0.200923	1.099726	1.281606
16	6	0	-2.612256	3.003157	1.472828
17	1	0	-3.995530	3.321666	-0.150984
18	1	0	-1.056116	2.502119	2.879532
19	6	0	-1.893118	-1.524021	-0.532036
20	6	0	-3.067298	-1.673571	-1.281917
21	6	0	-1.928758	-1.818395	0.835983
22	6	0	-4.253743	-2.093731	-0.678591
23	1	0	-3.050738	-1.466054	-2.349565
24	6	0	-3.111850	-2.244359	1.442122
25	1	0	-1.015962	-1.725180	1.414784
26	6	0	-4.279555	-2.380466	0.688127
27	1	0	-5.153946	-2.205443	-1.276488
28	1	0	-3.121250	-2.473344	2.504267
29	6	0	2.859846	-0.671158	-0.153364
30	6	0	3.207399	-1.740813	0.687149
31	6	0	3.849481	0.249035	-0.530344
32	6	0	4.513490	-1.880492	1.148536
33	1	0	2.438071	-2.451430	0.967852
34	6	0	5.158653	0.104878	-0.068513
35	1	0	3.600131	1.071575	-1.191599
36	6	0	5.494164	-0.957173	0.772753
37	1	0	4.768653	-2.709559	1.802001
38	1	0	5.917223	0.820950	-0.370617
39	1	0	2.879242	3.487372	-0.067099
40	1	0	2.049822	4.011858	-1.365835
41	1	0	1.270806	3.715377	0.032993
42	7	0	2.007307	3.368443	-0.578213
43	1	0	6.513097	-1.067265	1.132106
44	1	0	-3.160915	3.625000	2.174117
45	1	0	-5.199704	-2.713789	1.159456

9



Thermodynamic quantities at 298.15K and 1.00 atm		
Electronic Energy (E)	-5071634.773	$kJ \cdot mol^{-1}$
Enthalpy (H)	-5070634.157	$kJ \cdot mol^{-1}$
Gibbs free energy (G)	-5070890.269	$kJ \cdot mol^{-1}$
ZPVE	921.879	$kJ \cdot mol^{-1}$
Correction to U	998.137	$kJ \cdot mol^{-1}$
Correction to H	1000.615	$kJ \cdot mol^{-1}$
Correction to G	744.504	$kJ \cdot mol^{-1}$
S_{total}	859.025	$J \cdot mol^{-1} \cdot K^{-1}$
S_{vib}	510.189	$J \cdot mol^{-1} \cdot K^{-1}$

Center Number	Atomic Number	Atomic type	Cartesian Coordinates (Angstroms) X	Y	Z
1	6	0	-0.380521	0.423475	0.642663
2	6	0	-0.449421	-0.542520	-0.608654
3	6	0	1.702183	-0.106105	0.078435
4	1	0	-0.722637	-0.132589	1.526856
5	1	0	-0.669640	0.054021	-1.504418
6	7	0	0.940980	-1.016935	-0.648031
7	1	0	1.296690	-1.311093	-1.550042
8	7	0	1.048171	0.722492	0.819338
9	6	0	-1.477493	-1.646004	-0.493270
10	6	0	-2.721494	-1.508232	-1.121080
11	6	0	-1.225693	-2.798319	0.264684
12	6	0	-3.701129	-2.491188	-0.988550
13	1	0	-2.926036	-0.627765	-1.723210
14	6	0	-2.196474	-3.786623	0.396234
15	1	0	-0.256977	-2.923598	0.736679
16	6	0	-3.438368	-3.633179	-0.229544
17	1	0	-4.658751	-2.376563	-1.483952
18	1	0	-1.988153	-4.679904	0.975455
19	6	0	-1.245973	1.657774	0.494240
20	6	0	-2.570936	1.649824	0.949045
21	6	0	-0.753642	2.808535	-0.134135
22	6	0	-3.392690	2.760851	0.770970
23	1	0	-2.964557	0.767995	1.446014
24	6	0	-1.566408	3.925558	-0.310179
25	1	0	0.275755	2.827137	-0.475775
26	6	0	-2.890188	3.901065	0.138456
27	1	0	-4.419082	2.741158	1.120988
28	1	0	-1.176587	4.811600	-0.799295
29	6	0	3.179367	-0.153206	0.023873
30	6	0	3.920823	0.943002	0.490704
31	6	0	3.854120	-1.273374	-0.481796
32	6	0	5.309519	0.923275	0.444811
33	1	0	3.392815	1.805002	0.881632
34	6	0	5.246132	-1.295761	-0.527990
35	1	0	3.297652	-2.140422	-0.820869
36	6	0	5.973945	-0.196630	-0.067963
37	1	0	5.877760	1.777158	0.796564
38	1	0	5.762769	-2.163735	-0.921600
39	6	0	-3.755092	5.120752	-0.003898
40	6	0	-4.501165	-4.677472	-0.038569
41	6	0	7.477396	-0.239455	-0.067433
42	9	0	7.963136	-1.030975	-1.050190
43	9	0	7.965247	-0.724673	1.100760
44	9	0	8.018725	0.988543	-0.232964
45	9	0	-5.193503	-4.489013	1.113242
46	9	0	-3.979671	-5.924889	0.028332
47	9	0	-5.409002	-4.674316	-1.040818
48	9	0	-3.399822	5.875068	-1.069647
49	9	0	-5.061923	4.802461	-0.154803
50	9	0	-3.679054	5.928805	1.083743

8. Crystallography

Data for Compound **1** were collected on a Bruker X8 prospector diffractometer with an Apex II CCD detector and a Incoatec IμS 1.0 CuK_α Microfocus Source, at a temperature of 150 K on and reduced using CrysAlisPro 171.39.21a.[5] Data for Compound **2** and **5** were collected on a dual source Rigaku FR-X rotating anode diffractometer using MoK_α wavelength, at a temperature of 150K and reduced using CrysAlisPro 171.39.21a.[5] The structures were solved and refined using Shelx-2016 implemented through Olex2 v1.2.8.[6,7] Data for Compound **9** were collected on a dual source Rigaku FR-X rotating anode diffractometer using CuK_α wavelength, at a temperature of 150K and reduced using CrysAlisPro 171.39.21a.[5] The structure was solved and refined using Shelx-2016 implemented through Olex2 v1.2.8.[6,7] All plots were produced using PLATON.[8]

Table S3 Crystallographic information for Compound **1**

Identification code	s4860x
Empirical formula	$C_{24}H_{15}F_9N_2$
Formula weight	502.38
Temperature/K	150
Crystal system	tetragonal
Space group	$P4_3$
a/Å	10.9162(2)
b/Å	10.9162(2)
c/Å	19.1285(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2279.42(10)
Z	4
ρ_{calc}g/cm^3	1.464
μ/mm^{-1}	1.228
F(000)	1016.0
Crystal size/mm^3	0.254 × 0.233 × 0.132
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.1 to 136.488
Index ranges	$-12 \leq h \leq 13$, $-12 \leq k \leq 13$, $-23 \leq l \leq 23$
Reflections collected	26788
Independent reflections	4163 [R_{int} = 0.0387, R_{sigma} = 0.0166]
Data/restraints/parameters	4163/2/329
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0480, wR_2 = 0.1231
Final R indexes [all data]	R_1 = 0.0519, wR_2 = 0.1271
Largest diff. peak/hole / e Å^{-3}	0.36/-0.28
Flack parameter	0.0(2)

Table S4 Crystallographic information for Compound **2**

Identification code	s4935l
Empirical formula	$C_{30}H_{42}N_5$ (Main molecule)
Formula weight	472.34
Temperature/K	199.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.1338(3)
b/Å	30.1549(9)
c/Å	18.5852(5)
α/°	90
β/°	91.647(2)
γ/°	90
Volume/Å^3	7917.8(4)
Z	8
ρ_{calc}g/cm^3	1.503
μ/mm^{-1}	2.401
F(000)	3505.0
Crystal size/mm^3	0.275 × 0.058 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.478 to 52.87
Index ranges	$-17 \leq h \leq 17$, $-35 \leq k \leq 37$, $-23 \leq l \leq 23$
Reflections collected	51690
Independent reflections	16200 [R_{int} = 0.0492, R_{sigma} = 0.0612]
Data/restraints/parameters	16200/20/814
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0484, wR_2 = 0.1339
Final R indexes [all data]	R_1 = 0.0907, wR_2 = 0.1497
Largest diff. peak/hole / e Å^{-3}	1.67/-0.71

Table S5 Crystallographic information for Compound **5**

Identification code	s4866l
Empirical formula	$C_{21}H_{15}F_{15}N_2S_3$
Formula weight	676.53
Temperature/K	150.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.2146(2)
b/Å	9.99845(16)
c/Å	20.3665(3)
α/°	90
β/°	91.4162(15)
γ/°	90
Volume/Å^3	2486.54(7)
Z	4
ρ_{calc}g/cm^3	1.807
μ/mm^{-1}	0.428
F(000)	1352.0
Crystal size/mm^3	0.402 × 0.375 × 0.209
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.538 to 52.744
Index ranges	$-15 \leq h \leq 15$, $-12 \leq k \leq 12$, $-23 \leq l \leq 25$
Reflections collected	27722
Independent reflections	5087 [R_{int} = 0.0241, R_{sigma} = 0.0169]
Data/restraints/parameters	5087/0/430
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0373, wR_2 = 0.0929
Final R indexes [all data]	R_1 = 0.0426, wR_2 = 0.0963
Largest diff. peak/hole / e Å^{-3}	0.37/-0.72

Table S6 Crystallographic information for Compound **9**

Identification code	s4980l
Empirical formula	$C_{24}H_{15}F_9N_2$
Formula weight	502.38
Temperature/K	150.03(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	10.08130(17)
b/Å	20.6490(4)
c/Å	21.8088(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4539.89(14)
Z	8
ρ_{calc}g/cm^3	1.470
μ/mm^{-1}	1.233
F(000)	2032.0
Crystal size/mm^3	0.144 × 0.058 × 0.022
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.108 to 136.47
Index ranges	-11 ≤ h ≤ 12, -23 ≤ k ≤ 24, -26 ≤ l ≤ 26
Reflections collected	16281
Independent reflections	4146 [R_{int} = 0.0282, R_{sigma} = 0.0285]
Data/restraints/parameters	4146/418/442
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0705, wR_2 = 0.1874
Final R indexes [all data]	R_1 = 0.0793, wR_2 = 0.1952
Largest diff. peak/hole / e Å^{-3}	0.56/-0.74

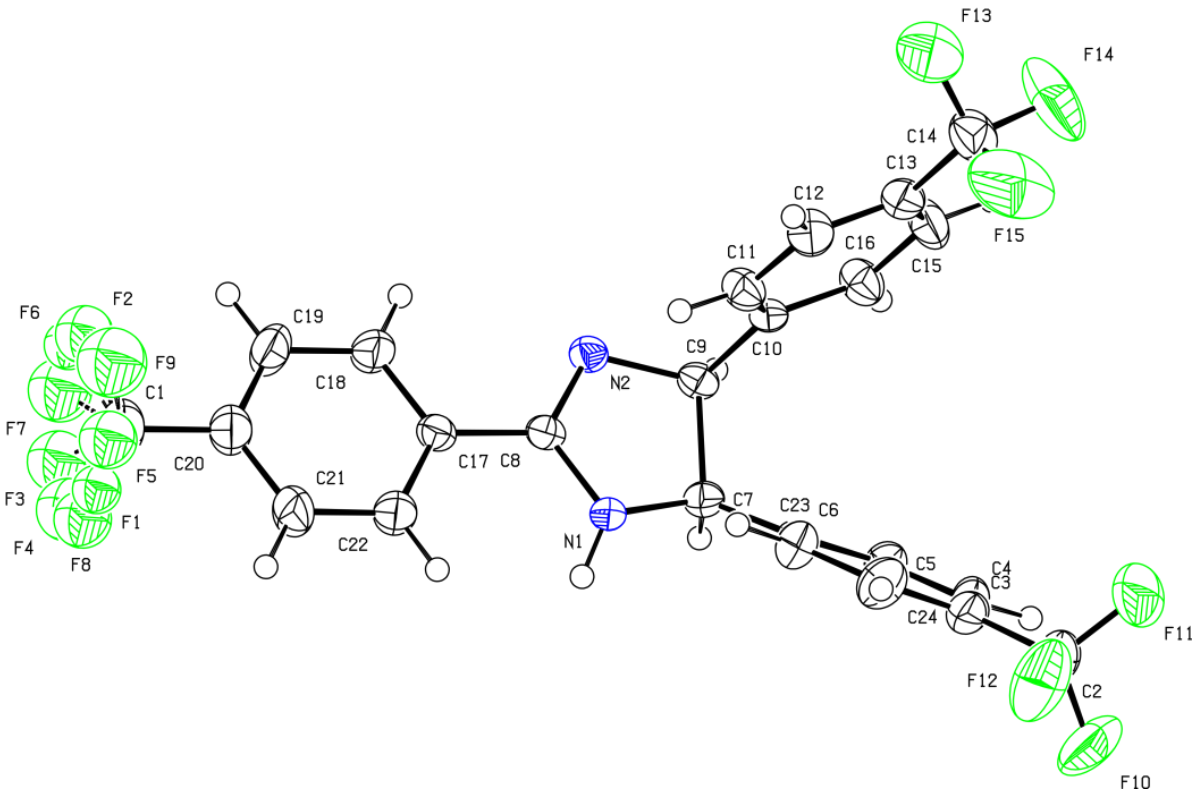


Fig. S114 ORTEP plot unit of Compound **1** in the crystal (Ellipsoids 50% probability).

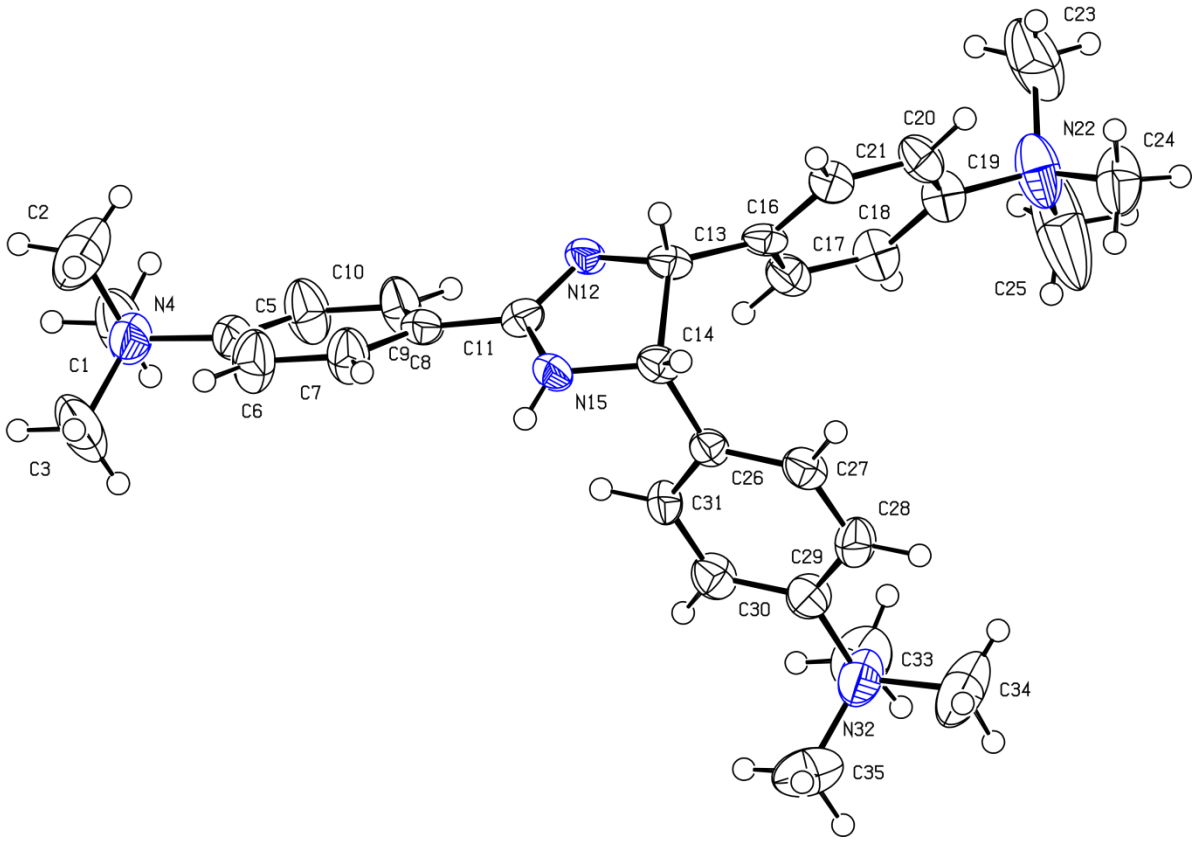


Fig. S115 ORTEP plot of one of the main molecule moieties of Compound **2** in the crystal (Ellipsoids 50% probability). Second main molecule moiety, iodide and water omitted for clarity.

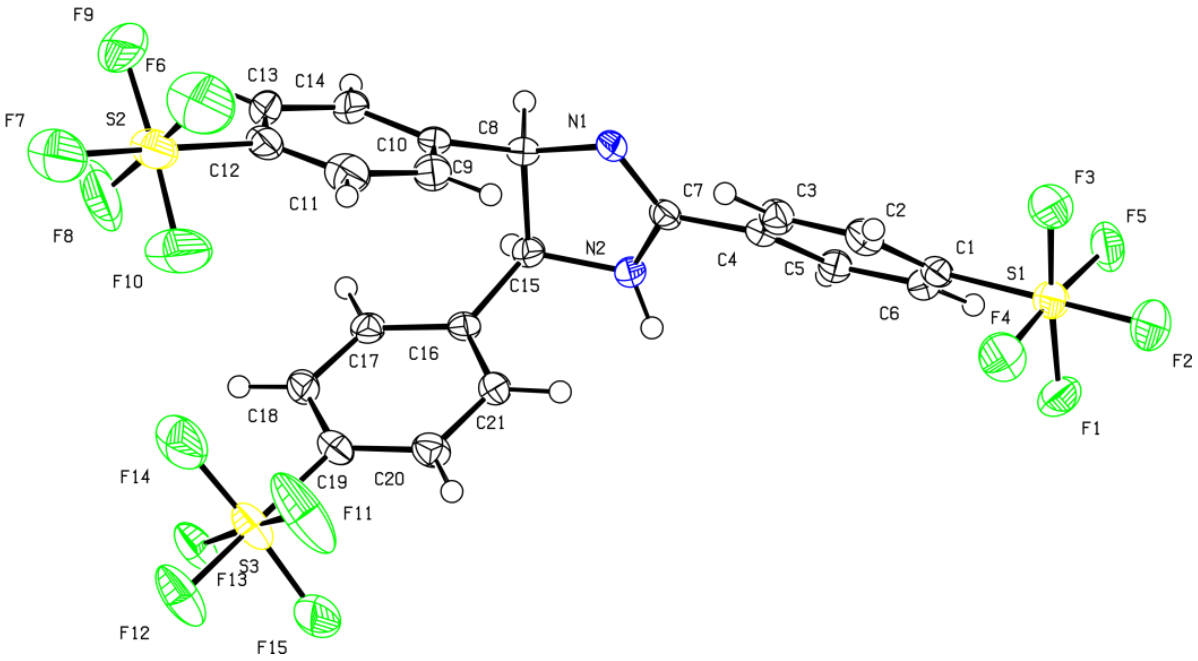


Fig. S116 ORTEP plot unit of Compound **5** in the crystal (Ellipsoids 50% probability).

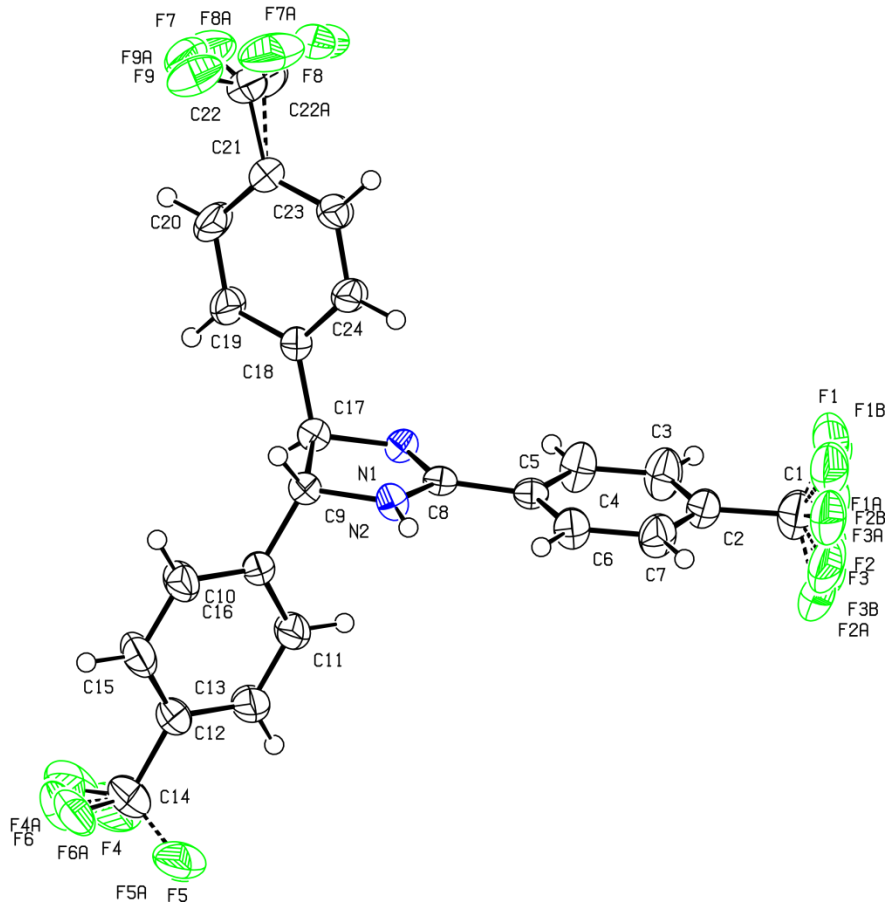


Fig. S117 ORTEP plot of Compound **9** in the crystal (Ellipsoids 50% probability).

9. Membrane separation

Table S7 Obtained flux and rejection values for GMT-oNF1, GMT-oNF2, NF030306 and Duramem® at different pressures.

	Flux ($L\ m^{-2}\ h^{-1}$)	Rejection of **1** (%)	Rejection of Impurity (%)
		GMT-oNF1	
10 bar	50.21 ± 1.32	83.52 ± 0.18	11.03 ± 1.01
20 bar	87.49 ± 0.43	84.57 ± 0.16	15.71 ± 0.29
30 bar	113.05 ± 1.50	84.06 ± 0.14	19.12 ± 0.16
		GMT-oNF2	
10 bar	57.95 ± 1.27	85.23 ± 0.30	10.72 ± 1.04
20 bar	107.30 ± 2.49	84.49 ± 0.32	14.96 ± 0.51
30 bar	135.93 ± 2.17	82.81 ± 0.07	18.94 ± 0.17
		NF030306	
10 bar	3.13 ± 0.11	88.71 ± 0.17	42.98 ± 0.81
20 bar	7.15 ± 0.16	93.38 ± 0.09	51.06 ± 0.70
30 bar	11.68 ± 0.30	96.03 ± 0.05	51.15 ± 0.86
40 bar	19.22 ± 0.12	95.96 ± 0.05	37.04 ± 1.67
		Duramem 300	
10 bar	2.53 ± 0.10	99.33 ± 0.01	58.62 ± 0.53
20 bar	5.52 ± 0.04	99.80 ± 0.01	68.42 ± 0.23
30 bar	7.75 ± 0.16	99.75 ± 0.02	73.78 ± 0.26
40 bar	8.37 ± 0.16	99.08 ± 0.14	76.45± 0.46

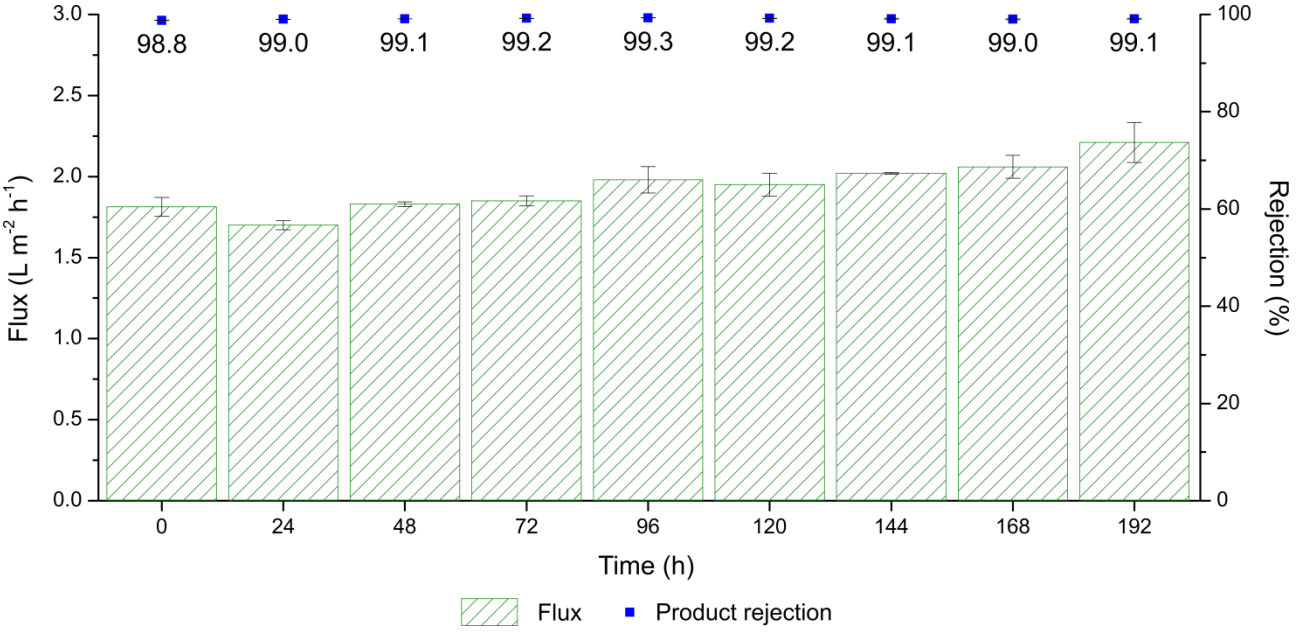


Fig. S118 Long term stability of Duramem 300 membrane at 20 bar.

Mathematical framework of diafiltration

To draw up the mathematical framework of diafiltration, the concept of rejection should be laid down. By definition, the rejection of a solute is the relative concentration decrease between the two sides of the membrane, usually expressed in percentage as the following:

$$R_{\mathrm{i}} = 100\% \cdot \left(\frac{C_{\mathrm{R,i}} - C_{\mathrm{P,i}}}{C_{\mathrm{R,i}}}\right) = 100\% \cdot \left(1 - \frac{C_{\mathrm{P,i}}}{C_{\mathrm{R,i}}}\right) \qquad (5)$$

Where R_{i} is the rejection of the solute in percentage, $C_{\mathrm{R,i}}$ and $C_{\mathrm{P,i}}$ are the concentrations of the solute in the retentate and permeate, respectively, usually given in g L^{-1}.

The schematic system setup used for the process modelling is illustrated in **Fig. S119**. In all cases, it was assumed that the system operates at constant volume. The mixing was assumed to be perfect in each stage. The separation was modelled for a two compound mixture of **1** and its starting material impurity. The initial concentrations in the feed, the rejection values and the flux from the first stage were obtained from experimental data.

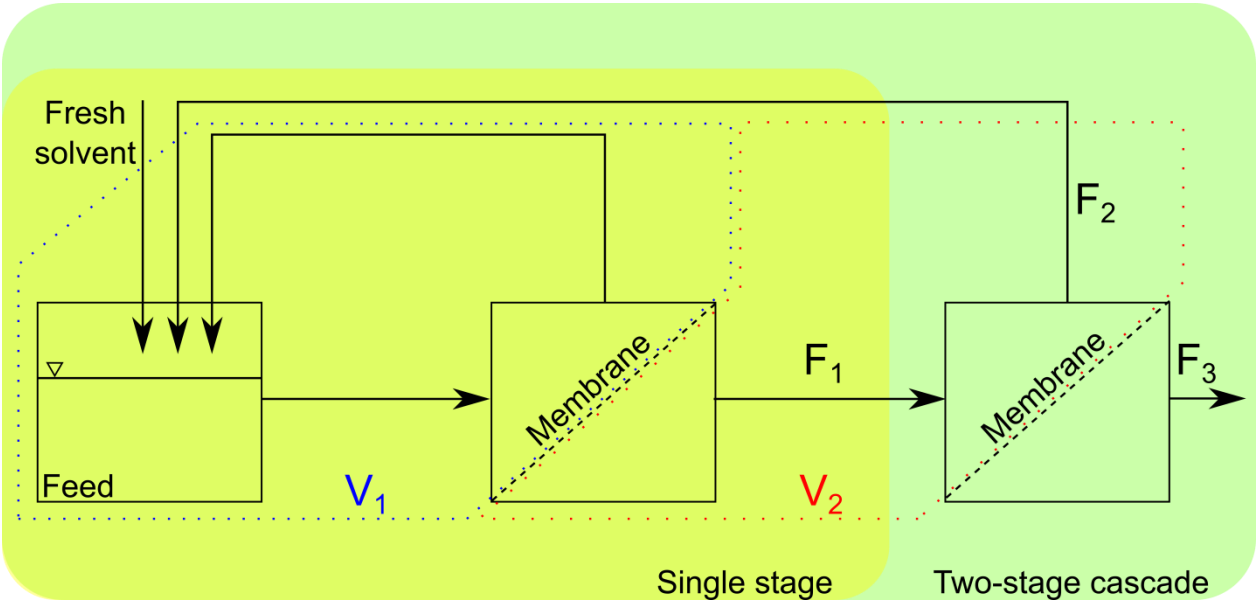


Fig. S119 Schematic system setup used for the process modelling. The yellow and green areas show the single stage and the two-stage setups, respectively. F_1 represents the permeate flow rate from the first stage, while F_3 is the permeate flow rate from the second stage. F_2 shows the flow rate of the recycle line from the second stage. V_1 and V_2 are the system volumes for the first and second stage, respectively.

Single stage

Using the above described experimental parameters and assumptions, mass balances for both compounds can be written around the system as the followings:

$$\frac{dC_{\mathrm{R,i}}}{dt} = -\frac{C_{\mathrm{R,i}} \cdot (1 - \frac{R_{\mathrm{i}}}{100\%}) \cdot F_1}{V_1} \quad (6)$$

$$\frac{dC_{\mathrm{R,j}}}{dt} = -\frac{C_{\mathrm{R,j}} \cdot (1 - \frac{R_{\mathrm{j}}}{100\%}) \cdot F_1}{V_1} \quad (7)$$

Where $C_{\mathrm{R,i}}$ and $C_{\mathrm{R,j}}$ are the concentrations of **1** and the impurity, respectively, in the retentate in g L^{-1}; R_{i} and R_{j} are the rejections of **1** and the impurity, respectively given in percentage; F_1 is the flow rate of the permeate in L h^{-1} and V_1 is the system volume in L.

Applying the initial concentrations, these differential equations can be easily solved using a Runge-Kutta numerical method in MATLAB[2]. The solution gives the concentrations in the function of time. Normalised concentration values of a solute can be obtained after dividing with the initial concentration. The yield of **1** is its normalised concentration expressed in percentage. The purity of **1** was calculated as the following:

$$P_{\mathrm{i}} = \frac{C_{\mathrm{R,i}}}{C_{\mathrm{R,i}} + C_{\mathrm{R,j}}} \cdot 100\% \quad (8)$$

Where P_{i} is the purity of **1** in percentage. The obtained normalised concentrations and purity values were plotted against the number of diavolumes. The number of diavolumes is a dimensionless time-like parameter indicating the progress of the filtration and it was calculated as the following:

$$Dv = \frac{F_1 \cdot t}{V_1} \quad (9)$$

Where *Dv* is the number of diavolumes and *t* is the filtration time in hours.

Two-stage cascade

Although OSN has been around since the late 20th century, organic solvent nanofiltration cascades have been gaining attention only in recent years. These configurations featuring more than one stage have been proposed to increase the efficiency[9] and the sustainability[10] of a membrane process or for solvent recovery[11]. The mathematical description of two-stage cascades has been drawn up in these works.[9-11] An important detail of the description is the introduction of recycle ratio (r_C). This dimensionless parameter is defined as the flow rate ratio of the first stage permeate (F_1) and the recycle line (F_2) as in **Fig. S119**. Using r_C, all flow rates in the system can be given as the function of F_1.

Similarly to the single stage, mass balances for both compounds can be written around both stages of the system using the above described experimental parameters and assumptions:

$$\frac{dC_{1,\mathrm{i}}}{dt} = \frac{C_{2,\mathrm{i}} \cdot r_\mathrm{C} \cdot F_1 - C_{1,\mathrm{i}} \cdot (1 - \frac{R_{1,\mathrm{i}}}{100\%}) \cdot F_1}{V_1} \tag{10}$$

$$\frac{dC_{1,\mathrm{j}}}{dt} = \frac{C_{2,\mathrm{j}} \cdot r_\mathrm{C} \cdot F_1 - C_{1,\mathrm{j}} \cdot (1 - \frac{R_{1,\mathrm{j}}}{100\%}) \cdot F_1}{V_1} \tag{11}$$

$$\frac{dC_{2,\mathrm{i}}}{dt} = \frac{C_{1,\mathrm{i}} \cdot (1 - \frac{R_{1,\mathrm{i}}}{100\%}) \cdot F_1 - C_{2,i} \cdot \left(1 - \frac{R_{2,i}}{100\%}\right) \cdot (1 - r_\mathrm{C}) \cdot F_1 - C_{2,\mathrm{i}} \cdot r_\mathrm{C} \cdot F_1}{V_2} \tag{12}$$

$$\frac{dC_{2,\mathrm{j}}}{dt} = \frac{C_{1,j} \cdot (1 - \frac{R_{1,\mathrm{j}}}{100\%}) \cdot F_1 - C_{2,\mathrm{j}} \cdot \left(1 - \frac{R_{2,\mathrm{j}}}{100\%}\right) \cdot (1 - r_\mathrm{C}) \cdot F_1 - C_{2,\mathrm{j}} \cdot r_\mathrm{C} \cdot F_1}{V_2} \tag{13}$$

Where $C_{1,\mathrm{i}}$ and $C_{2,\mathrm{i}}$ are the concentrations of **1** in the first stage and second stage, respectively, in g L^{-1}; $C_{1,\mathrm{j}}$ and $C_{2,\mathrm{j}}$ are the concentrations of the starting material impurity in the first stage and second stage, respectively, in g L^{-1}; $R_{1,\mathrm{i}}$ and $R_{2,\mathrm{i}}$ are the rejections of **1** on the first and second membrane, respectively, given in percentage; $R_{1,\mathrm{j}}$ and $R_{2,\mathrm{j}}$ are the rejections of the impurity on the first and second membrane, respectively, given in percentage; r_C is the recycle ratio; F_1 is the flow rate of the first-stage permeate in L h^{-1} and V_1 and V_2 are the system volumes of the stages in L.

In our case, the modelled two-stage cascade consists of two identical membrane units. Therefore, $R_{1,\mathrm{i}}$ equals $R_{2,\mathrm{i}}$; $R_{1,\mathrm{j}}$ equals $R_{2,\mathrm{j}}$; and V_1 equals V_2. For the simulations, a convenient value of 0.5 was selected for r_C[10]. Applying the initial concentrations, these differential equations can be easily solved using a Runge-Kutta numerical method in MATLAB[2]. The solution gives the concentrations in the function of time. As V_1 equals V_2 and there is no solute in the second stage at the beginning of the diafiltration, normalised concentrations (N) for the whole system can be obtained as the followings:

$$N_\mathrm{i} = \frac{C_{1,\mathrm{i}} \cdot V_1 + C_{2,\mathrm{i}} \cdot V_2}{C_{1,\mathrm{i}}^{t=0} \cdot V_1 + C_{2,\mathrm{i}}^{t=0} \cdot V_2} = \frac{C_{1,\mathrm{i}} + C_{2,\mathrm{i}}}{C_{1,\mathrm{i}}^{t=0}} \tag{14}$$

$$N_\mathrm{j} = \frac{C_{1,\mathrm{j}} \cdot V_1 + C_{2,\mathrm{j}} \cdot V_2}{C_{1,\mathrm{j}}^{t=0} \cdot V_1 + C_{2,\mathrm{j}}^{t=0} \cdot V_2} = \frac{C_{1,\mathrm{j}} + C_{2,\mathrm{j}}}{C_{1,\mathrm{j}}^{t=0}} \tag{15}$$

Where $C^{t=0}$ is the initial concentration of a solute in the given stage. The yield of **1** is its normalised concentration expressed in percentage. The purity of **1** was calculated as the following:

$$P_{\mathrm{i}} = \frac{C_{1,\mathrm{i}} + C_{2,\mathrm{i}}}{C_{1,\mathrm{i}} + C_{2,\mathrm{i}} + C_{1,\mathrm{j}} + C_{2,\mathrm{j}}} \cdot 100\% \qquad (16)$$

Where P_{i} is the purity of **1** in percentage. The obtained normalised concentrations and purity values were plotted against the number of diavolumes. The number of diavolumes is a dimensionless time-like parameter indicating the progress of the filtration and it was calculated as the following:

$$Dv = \frac{F_1 \cdot (1 - r_{\mathrm{C}}) \cdot t}{V_1 + V_2} \qquad (17)$$

Where *Dv* is the number of diavolumes and *t* is the filtration time in hours. Comparing this equation with the one drawn up for a single stage, it is apparent that for reaching every diavolume, four times more time and double volume of solvent is required.

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