European Commission

Draft Assessment Report prepared according to the Commission Regulation (EU) N° 1107/2009

BAS 750F
(Mefentrifluconazole)

Volume 3 – B.2 (AS)

Rapporteur Member State: United Kingdom
Co-Rapporteur Member State: France & Austria

Version History

When	What
April 2017	Initial DAR

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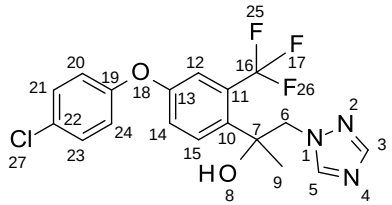
B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE

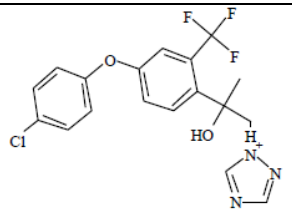
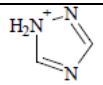
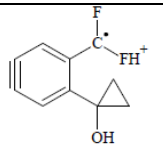
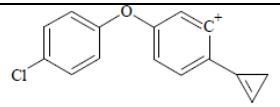
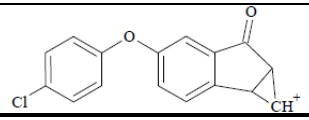
BAS 750 F is confirmed as the same as Reg.No. 5834378.

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.1. MELTING POINT AND BOILING POINT						
Melting, freezing or solidification point **B.2.1/01**	OPPTS 830.7200 DSC/TG method (equivalent to OECD 102 and EEC A.1)	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Melting point (onset): 126 °C	Acceptable Only the melting point of the purified active substance is required by Regulation (EC) 283/2013 The melting point is determined by differential thermal analysis and differential scanning calorimetry which is one of the methods described in both OECD 102 and EEC A.1	Y	[see 2014/1117052 Kroehl T. 2014 a]
		Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	Melting point (onset): 125 °C		Y	[see 2014/1117053 Kroehl T. 2014 b]
Boiling point **B.2.1/02**	OPPTS 830.7200 DSC/TG method (equivalent to OECD 103 and EEC A.2)	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Sample decomposed before boiling.	Acceptable Only the boiling point of the purified active substance is required by Regulation (EC) 283/2013 The boiling point is determined by differential thermal analysis and differential scanning calorimetry which is one of the methods described in both OECD 103 and EEC A.2 However, the boiling point could not be	Y	[see 2014/1117052 Kroehl T. 2014 a]
		Reg.No. 5834378 (TGAI) COD-001740: 98.8 %	Sample decomposed before boiling.		Y	[see 2014/1117053 Kroehl T. 2014 b]

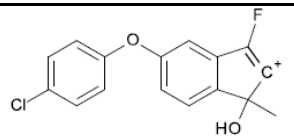
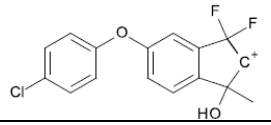
Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
				determined because of decomposition; the decomposition temperature is reported in Annex Point B.2.1/03 below.		
Decomposition / Sublimation temperature **B.2.1/03**	OPPTS 830.7200 DSC/TG method (equivalent to OECD 102)	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Decomposition temp. (onset): approx. 300 °C (onset of exothermic peak)	Acceptable Only the decomposition temperature of the purified active substance is required by Regulation (EC) 283/2013 The decomposition temperature is determined by differential thermal analysis and differential scanning calorimetry which is one of the methods described in both OECD 103 and EEC A.2	Y	[see 2014/1117052 Kroehl T. 2014 a]
		Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	Decomposition temp. (onset): approx. 300 °C (onset of exothermic peak)		Y	[see 2014/1117053 Kroehl T. 2014 b]
B.2.2. VAPOUR PRESSURE, VOLATILITY						
Vapour pressure **B.2.2/01**	OPPTS 830.7950 EEC A.4 OECD 104	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Vapour pressure: $p = 3.2 \cdot 10^{-6}$ Pa (20 °C) $p = 6.5 \cdot 10^{-6}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2014/1117052 Kroehl T. 2014 a]
Volatility (Henry's Law constant) **B.2.2/02**	Calculation	Calculated from vapour pressure and water solubility for Reg.No. 5834378 (PAI) Batch L84-238:	Henry Constant: $H = 1.6 \cdot 10^{-3}$ Pa $\cdot$ m^3 $\cdot$ mol^{-1}	Acceptable Moderately volatile	N	[see 2014/1173597 Kroehl T. 2014 c]

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td>99.7 %</td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="7">B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)</td></tr>
<tr><td rowspan="2">Physical state and colour
B.2.3/01</td><td rowspan="2">OPPTS 830.6302 to 830.6304 (visual and olfactory examination)</td><td>Reg.No. 5834378 (PAI)
Batch L84-238: 99.7 %</td><td>white, solid and odourless crystalline powder</td><td>Acceptable</td><td>Y</td><td>[see 2014/1117052 Kroehl T. 2014 a]</td></tr>
<tr><td>Reg.No. 5834378 (TGAI)
Batch COD-001740: 98.8 %</td><td>fine powdered, off-white solid of moderate thiolic odour</td><td>Acceptable</td><td>Y</td><td>[see 2014/1117053 Kroehl T. 2014 b]</td></tr>
<tr><td colspan="7">B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY</td></tr>
<tr><td>Ultraviolet/visible (UV/VIS)
B.2.4/01</td><td>OECD 101, UV VIS</td><td>Reg.No. 5834378 (PAI)
Batch L84-238: 99.7 %</td><td>molar extinction coefficients ε in L · mol^{-1} · cm^{-1} (at relevant wavelengths)
<table>
<tr><th></th><th>Methanol solution
(pH 6.3)</th><th>Methanol/Water solution
10:90
(pH 6.4)</th><th>Methanol/HCl (1M)/Water solution
10:5:85
(pH 1.4)</th><th>Methanol/NaOH (1M)/Water solution
10:5:85
(pH 12.2)</th></tr>
<tr><td>Main peak</td><td>37761 (202 nm)</td><td>54636 (194 nm)</td><td>43245 (199 nm)</td><td>16668 (231 nm)</td></tr>
<tr><td>Shoulder peaks</td><td>17322 (232 nm)
2774 (272 nm)
1727 (290 nm)
439 (295 nm)</td><td>16618 (231 nm)
2780 (275 nm)
1504 (290 nm)
420 (295 nm)</td><td>16553 (231 nm)
2759 (272 nm)
1438 (290 nm)
402 (295 nm)</td><td>2784 (277 nm)
1653 (290 nm)
615 (295 nm)</td></tr>
</table>
</td><td>Acceptable
As BAS 750 F absorbs at wavelengths > 290 nm for all pHs tested, there is potential for photolytic degradation.
However BAS 750 F only absorbs at wavelengths <313 nm for all pHs tested, therefore testing for phytotoxicity has not been triggered.</td><td>Y</td><td>[see 2014/1173598 Kroehl T., Behnken H. 2014 a]
[see 2015/1183750 Kroehl T. 2015 a]
[see 2016/1203119 Kroehl T. 2016 a]</td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
Infrared (IR) **B.2.4/02**	IR		wave numbers ῡ in cm^{-1} 3116 C-H stretching vibration in aromatic methine groups 2977 C-H stretching vibration in alkane groups 1484 C-C ring stretching in C-6 aromatic groups 1251 C-O stretching vibration in diaryl ethers 1158 C-O-C stretching vibration in ethers 1127 C-H rocking vibration in methyl groups 1087 C-O stretching vibration in alcohols 831 C-H stretching vibration in aromatic methine groups	Acceptable The spectrum is in accordance with the proposed structure		
Nuclear magnetic resonance (NMR) **B.2.4/03**	NMR		 Samples are dissolved in deuterated dimethyl sulfoxide (DMSO-d_6), shifts are given in ppm (assignments in brackets). **^{1}H**: 7.9 (**3**), 8.3 (**5**), 4.5 (**6**), 5.7 (**8**), 1.5 (**9**), 7.4 (**12**), 7.2 (**14**), 7.6 (**15**), 7.1 (**20**, **24**), 7.5 (**21**, **23**) **^{13}C**: 150.5 (**3**), 145.0 (**5**), 59.0 (**6**), 73.3 (**7**), 27.7 (**9**), 139.8 (**10**), 128.4[1] (**11**), 117.5[3] (**12**), 154.6 (**13**), 121.0 (**14**), 131.2 (**15**), 123.9[2] (**16**), 155.3 (**19**), 120.8 (**20**, **24**), 130.1 (**21**, **23**), 128.1 (**22**) [1] Quartet at 128.7, 128.5, 128.3 and 128.1 ppm due to $^{2}J_{C,F}$ coupling [2] Quartet at 126.7, 124.8, 123.0 and 121.2 ppm due to $^{1}J_{C,F}$ coupling [3] Quartet at 117.6, 117.5, 117.5 and 117.4 ppm due to $^{3}J_{C,F}$ coupling	Acceptable Extra peaks in ^{1}H NMR spectrum due to DMSO (2.5 ppm) and water (3.3 ppm) Extra peaks in ^{13}C NMR spectrum due to DMSO (39.5 ppm)		

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td>^{19}F: -53.1 (17, 25, 26)</td><td></td><td></td><td></td></tr>
<tr><td>Mass spectra (MS)
B.2.4/04</td><td>MS-ESI
GC/MS-EI
GC/MS-CI</td><td></td><td>Electrospray ionization (ESI):
m/z = 397.7 $[M+H]^+$
(protonated ion of BAS 750 F)
characteristic fragments of BAS 750 F:
m/z = 69.8, 182.0, 241.1, 269.0, 289.1, 309.1
<table>
<tr><th>m/z</th><th>Formula</th><th>Structure</th></tr>
<tr><td>397.7* $[M+H]^+$</td><td>$C_{18}H_{16}ClF_3N_3O_2(^+)$</td><td>  </td></tr>
<tr><td>69.8</td><td>$C_2H_4N_3(^+)$</td><td>  </td></tr>
<tr><td>182.0</td><td>$C_{10}H_8F_2O(*^+)$</td><td>  </td></tr>
<tr><td>241.1</td><td>$C_{15}H_{10}ClO$</td><td>  </td></tr>
<tr><td>269.0</td><td>$C_{16}H_{10}ClO_2(^+)$</td><td>  </td></tr>
</table></td><td>Acceptable</td><td></td><td></td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference

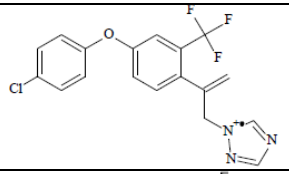
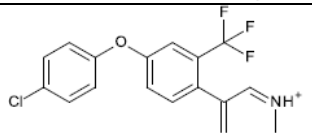
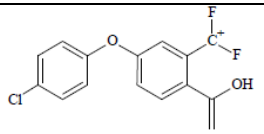
289.1	$C_{16}H_{11}ClFO_2(^+)$	
309.1	$C_{16}H_{12}ClF_2O_2(^+)$	

*The difference with the measured m/z to the calculated mass (*m/z* 398.1) is due to the intrinsic low mass accuracy of the used instrument. In the full scan, the deprotonated formate adduct $[M-H+HCOOH]^{-\cdot}$ was detected at *m/z* 442.1 which further demonstrates the validity of the assignment to BAS 750 F.

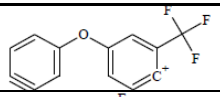
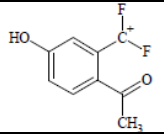
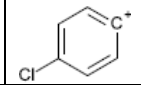
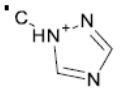
Electron ionization (EI):

m/z = 379 $[M-H_2O]^+$

characteristic fragments of BAS 750 F:
m/z = 83, 111, 185, 235, 295, 340

m/z	Formula	Structure
379	$C_{18}H_{13}ClF_3N_3O(*^+)$	
340	$C_{17}H_{14}ClF_3NO(^+)$	
295	$C_{15}H_{10}ClF_2O_2(^+)$	

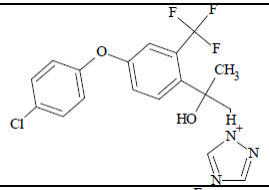
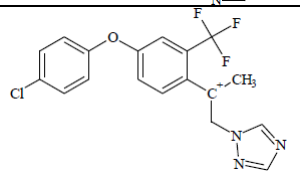
Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference

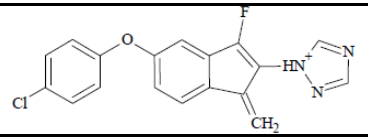
235	$C_{13}H_6F_3O(^+)$	
185	$C_9H_7F_2O_2(^+)$	
111	$C_6H_4Cl(^+)$	
83	$C_3H_5N_3(^{\bullet+})$	

Chemical ionization (CI):

m/z = 398 $[M]^+$

characteristic fragments of BAS 750 F
m/z = 340, 380

m/z	Formula	Structure
398	$C_{18}H_{16}ClF_3N_3O_2(^+)$	
380	$C_{18}H_{14}ClF_3N_3O(^+)$	

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td>340 | $C_{18}H_{12}ClFN_3O(^+)$ |  </td><td></td><td></td><td></td></tr>
<tr><td>Spectra for impurities
B.2.4/05</td><td></td><td></td><td></td><td>DMF has been identified by a GC/FID and GC/MS retention time match with a reference sample in Method APL0685/01 as evaluated in Volume 4 of this DAR and further spectroscopic methods were not deemed necessary for its identification.</td><td></td><td></td></tr>
<tr><td colspan="7">B.2.5. SOLUBILITY IN WATER</td></tr>
<tr><td>Solubility in water
B.2.5/01</td><td>EEC A.6
OECD 105
Analytical HPLC method (Study No. VP 048/2013)</td><td>Reg.No. 5834378 (PAI)
Batch L84-238: 99.7 %</td><td>Results were determined applying the column elution method at 20 °C.
<table>
<tr><th rowspan="2">Solvent medium</th><th colspan="3">Solubility (mg/L)</th></tr>
<tr><th>1st run</th><th>2nd run</th><th>Mean</th></tr>
<tr><td>water (pure water, resulting pH value: 6.8)</td><td>0.91</td><td>0.71</td><td>0.81</td></tr>
<tr><td>pH 4 (acetate buffer)</td><td>0.76</td><td>0.55</td><td>0.66</td></tr>
<tr><td>pH 7 (phosphate buffer)</td><td>0.66</td><td>0.76</td><td>0.71</td></tr>
</table></td><td>Acceptable

Slightly soluble in water (pure water, resulting pH value: 6.8), pH4 (acetate buffer) and pH7 (phosphate buffer).

The water solubility was determined in the acidic range (pH 4 to 5) as the pKa of the conjugate acid form present in acidic conditions is in the range 2-12 (3.0 ± 0.1).
The water solubility has not been determined in the alkaline range (pH 9 to 10) as the pKa of the non-ionised form present in alkaline conditions is</td><td>Y</td><td>[see 2013/1397136 Wilbrand S. 2013 a]
[see 2016/1203120 Kroehl T., 2016 b]</td></tr>
</table>

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td></td><td>outside of the range 2-12 (12.7 ± 0.3) therefore no dissociation is expected at pH 9 – 10.

The analytical HPLC method for the determination of the active substance was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR Volume 3 CA Section B.5 (Study No. VP 048/2013)</td><td></td><td></td></tr>
<tr><td colspan="7">B.2.6. SOLUBILITY IN ORGANIC SOLVENTS</td></tr>
<tr><td>Solubility in organic solvents
B.2.6/01</td><td>CIPAC MT 181
Analytical HPLC method (Study No. VP 048/2013)</td><td>Reg.No. 5834378 (TGAI)

Batch COD-001740: 98.8 %</td><td>
<table>
<tr><td>Solvent</td><td colspan="3">Solubility (mg/L)</td></tr>
<tr><td></td><td>1st run</td><td>2nd run</td><td>Mean</td></tr>
<tr><td>Acetone</td><td>92.7</td><td>93.7</td><td>93.2</td></tr>
<tr><td>Ethyl acetate</td><td>116.2</td><td>116.2</td><td>116.2</td></tr>
<tr><td>Methanol</td><td>75.2</td><td>71.2</td><td>73.2</td></tr>
<tr><td>1,2-Dichloroethane</td><td>55.3</td><td>55.4</td><td>55.3</td></tr>
<tr><td>Acetonitrile</td><td>49.3</td><td>49.5</td><td>49.4</td></tr>
<tr><td>Xylene</td><td>8.6</td><td>8.4</td><td>8.5</td></tr>
<tr><td>n-Heptane</td><td>0.0947</td><td>0.0944</td><td>0.0946</td></tr>
</table>
Results (in g/L) were obtained at 20 °C (± 0.5 °C) applying the flask method.
Acetone 93.2 (± 1.6)
Ethyl acetate 116.2 (± 1.8)
Methanol 73.2 (± 3.2)
1,2-Dichloroethane 55.3 (± 0.4)
Acetonitrile 49.4 (± 0.7)
Xylene 8.5 (± 0.1)
n-Heptane 9.46 · 10-2 (± 0.9 · 10-3)</td><td>Acceptable

Moderately soluble in acetone, ethyl acetate, methanol, 1,2-dichloroethane and acetonitrile.

Slightly soluble in xylene.

Very slightly soluble in n-heptane.

Although the solubility in aromatic hydrocarbon was not determined using toluene, which is stated as the preferred solvent in Reg. (EC) 283/2014; it was determined using xylene which is the preferred solvent in</td><td>Y</td><td>[see 2013/1391669 Wilbrand S. 2013 b]</td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
				CIPAC MT 181. Although the solubility in halogenated hydrocarbon was not determined using dichloromethane, which is stated as the preferred solvent in Reg. (EC) 283/2014; it was determined using 1,2,-dichloroethane which is the preferred solvent in CIPAC MT 181. The analytical HPLC method for the determination of the active substance was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR Volume 3 CA Section B.5 (Study No. VP 048/2013)		
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER						
Partition coefficient n-octanol/water B.2.7/01	EEC A.8 OECD 117	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Results determined at 20 °C applying the HPLC method. pH 4*: log P_{OW} = 3.4 pH 7: log P_{OW} = 3.4 pH 7*: log P_{OW} = 3.3 pH 9*: log P_{OW} = 3.4 * buffered	Acceptable According to EEC A.8, the HPLC method is applicable within the range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method). Pow <4 hence no need for additional risk assessment in other specialist areas for	Y	[see 2013/1382370 Wilbrand S. 2013 c]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
				potential to bioaccumulate.		
B.2.8. DISSOCIATION IN WATER						
Dissociation constant **B.2.8/01**	OECD 112	Reg.No. 5834378 (PAI) Batch L84-238: 99.7 %	Due to the low solubility of the test item in water, the titration method is not suitable for the determination of the dissociation constant. Instead of the titration method the spectrophotometric method was used in this study. In acidic and alkaline conditions, two different species of BAS 750 F are present, therefore there are two dissociation constants for BAS 750 F depending on pH. In acidic conditions, BAS 750 F is protonated at the triazole ring and the dissociation constant refers to the loss of this proton. In alkaline conditions, the BAS 750 F is present in its non-ionised form and the dissociation constant refers to the loss of the hydroxyl proton. The following pKas correspond to the conjugate acid form present in acidic conditions. pK_a at 20 °C: 2.7 ± 0.5 pK_a at 30 °C: 2.5 ± 0.5 pK_a (calculated; ACD Lab 12.01): 3.0 ± 0.1 Due to the high variation of the test results within each measurement as well as to the high relative standard deviations, the pKa value calculated is reported as the final result of the dissociation constant of Reg. No. 5834378. Therefore limited dissociation is expected to occur at pH 4-5. The following pKa corresponds to the non-ionized form present in alkaline conditions: pK_a (calculated; ACD Lab 12.01): 12.7 ± 0.3. Therefore no dissociation is expected at pH 9-10.	Acceptable	Y	[see 2013/1397719 Wilbrand S. 2013 d]
B.2.9. FLAMMABILITY AND SELF-HEATING						
Flammability **B.2.9/01**	EEC A.10	Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	Flammability: No ignition of the test item by flame in the preliminary test (the test item melted). Thus, the main test was omitted.	Acceptable EEC A10 deemed sufficiently comparable to Test N.1 as described in Section 33.2.1 of the UN Recommendations on the Transport of Dangerous Goods used	Y	[see 2014/1109962 Moeller M. 2014 a]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
				for classification of flammability. BAS 750 F is not classified as a flammable solid under the CLP regulation.		
Self heating **B.2.9/02**	EEC A.16	Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	Relative self-ignition of solids: Test not performed (melting point approximately 110 °C (< 160 °C)).	Acceptable Self heating was not observed up to the melting point reported in Annex point B.2.1/01	Y	[see 2014/1109962 Moeller M. 2014 a]
B.2.10. FLASH POINT						
Flash point **B.2.10/01**			Not applicable as Reg.No. 5834378 is a solid (melting point > 40 °C).	Acceptable	Y	[see 2014/1109962 Moeller M. 2014 a]
B.2.11. EXPLOSIVE PROPERTIES						
Explosive properties **B.2.11/01**	OECD 113 EEC A.14	Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	Thermal Stability (DSC method): 1st reaction: onset 110 °C, energy intake 110 J/g (endothermic) 2nd reaction: onset 340°C, energy release 580 J/g (exothermic) Mechanical sensitivity, friction: No reaction observed in six tests using BAM friction apparatus with a force of 360 N. Mechanical sensitivity, impact. No reaction observed in six tests using BAM drop hammer (mass 10 kg, drop height 40 cm).	Acceptable Test method EEC A14 is considered comparable to test methods described in Part I of the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria for classification of explosive substances by CLP. BAS 750 F is not classified as an explosive substance according to GHS or CLP Regulation EC 1272/2008 Annex 1:	Y	[see 2014/1109962 Moeller M. 2014 a]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			Thermal sensitivity, Koenen-test: The results of the test series with a 2.0 mm diameter orifice plate showed no explosion. Therefore, further tests were not required. Final conclusion: not explosive	2.1.		
B.2.12. SURFACE TENSION						
Surface tension **B.2.12/01**	OECD 115		Not applicable, substances with a water solubility < 1 mg/L need not be tested.	Acceptable		
B.2.13. OXIDISING PROPERTIES						
Oxidizing properties **B.2.13/01**	EEC A.17	Reg.No. 5834378 (TGAI) Batch COD-001740: 98.8 %	The highest burning rate of a test mixture of test item with cellulose (1.07 mm/s) is lower than the highest burning rate of a mixture of barium nitrate with cellulose (1.27 mm/s). Conclusion: Not oxidizing.	Acceptable EEC A17 deemed sufficiently comparable to Test O1 as described in Section 34.4.1 of the UN Recommendations on the Transport of Dangerous Goods used for classification of oxidising solids. BAS 750 F is not classified as an *oxidising solid* according to GHS or CLP Regulation EC 1272/2008 Annex 1.	Y	[see 2014/1109962 Moeller M. 2014 a]
B.2.14. OTHER STUDIES						
Vapour pressure of the metabolites **M750F003 (Reg.No. 5924326)** **M750F005 (Reg.No.**	EEC A.4 OECD 104	Reg.No. 5924326, L84-250: 99.6 %	M750F003 (Reg.No. 5924326): $p = 3.4 \cdot 10^{-06}$ Pa (20 °C) $p = 7.1 \cdot 10^{-06}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2015/1205970 Daum A. 2015 a]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
6003433) **M750F006 (Reg.No. 5863469)** **M750F007 (Reg.No. 6003432)** **M750F008 (Reg.No. 6010286)**		Reg.No. 6003433, L87-34: 99.4 %	<u>M750F005 (Reg.No. 6003433):</u> $p = 2.3 \cdot 10^{-09}$ Pa (20 °C) $p = 6.1 \cdot 10^{-09}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2015/1205971 Daum A. 2015 b]
		Reg.No. 5863469, L87-30: 98.9 %	<u>M750F006 (Reg.No. 5863469):</u> $p = 4.5 \cdot 10^{-08}$ Pa (20 °C) $p = 1.0 \cdot 10^{-07}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2015/1205972 Daum A. 2015 c]
		Reg.No. 6003432, L87-32-1: 97.0 %	<u>M750F007 (Reg.No. 6003432):</u> $p = 3.7 \cdot 10^{-11}$ Pa (20 °C) $p = 1.0 \cdot 10^{-10}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2015/1205973 Daum A. 2015 d]
		Reg.No. 6010286, L85-94: 96.5 %	<u>M750F008 (Reg.No. 6010286):</u> $p = 2.7 \cdot 10^{-13}$ Pa (20 °C) $p = 9.1 \cdot 10^{-13}$ Pa (25 °C)	Acceptable Very slightly volatile	Y	[see 2015/1205976 Daum A. 2015 e]
Water solubility of the metabolites **M750F003 (Reg.No. 5924326)** **M750F005 (Reg.No. 6003433)** **M750F006 (Reg.No. 5863469)** **M750F007 (Reg.No. 6003432)** **M750F008 (Reg.No. 6010286)**	EEC A.6 OECD 105 HPLC method for the determination of Reg.No. 5924326 (Study no. VP 028/2015)	Reg.No. 5924326, L84-250: 99.6 %	<u>M750F003 (Reg.No. 5924326): Flask method (solubility > 0.01 g/L)</u> Double Distilled Water 2.46 (± 0.04) g/L, pH 6.5 Acetate Buffer 2.42 (± 0.11) g/L, pH 4.4 Borate Buffer 2.48 (± 0.03) g/L, pH 8.3* *the pH of the buffer solution without test item was 8.92 Note: pH values reflect average values of the saturated solutions. Determinations of water solubility were performed at 20 (±0.5) °C.	Acceptable Readily soluble in double distilled water, acetate buffer and borate buffer The HPLC method for the quantification of the concentration of the metabolite was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR CA Volume 3 Section B.5 (Study no. VP 028/2015).	Y	[see 2015/1139989 Wilbrand S. 2015 a] [see 2015/1252305 Wilbrand S. 2016 a] see 2016/1030230 Wilbrand S. 2016 b]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	EEC A.6 OECD 105 HPLC method for the determination of Reg.No. 6003433 (Study no. VP 029/2015)	Reg.No. 6003433, L87-34: 99.4 %	<u>M750F005 (Reg.No. 6003433): Column elution method (solubility < 0.01 g/L)</u> Double Distilled Water 11.3 (± 0.6) mg/L, pH 6.8 Acetate Buffer 9.9 (± 1.5) mg/L, pH 4.3 Borate Buffer 13.8 (± 1.3) mg/L, pH 9.0 Note: pH values reflect average values of the saturated solutions. Determinations of water solubility were performed at 20 (±0.5) °C.	Acceptable Slightly soluble in double distilled water, and borate buffer Moderately soluble in acetate buffer The HPLC method for the quantification of the concentration of the metabolite was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR CA Volume 3 Section B.5 (Study no. VP 029/2015)	Y	[see 2015/1139993 Wilbrand S. 2015 b]
	EEC A.6 OECD 105 HPLC method for the determination of Reg.No. 5863469 (Study no. VP 031/2015)	Reg.No. 5863469, L87-30: 98.9 %	<u>M750F006 (Reg.No. 5863469): Column elution method (solubility < 0.01 g/L)</u> Double Distilled Water 11.2 (± 1.3) mg/L, pH 7.1* Acetate Buffer 18.9 (± 2.4) mg/L, pH 4.2* Borate Buffer 13.9 (± 2.3) mg/L, pH 9.0 *pH-value of the buffer solution, used for the elution of the test item Note: unless otherwise flagged, pH values reflect average values of the saturated solutions. Determinations of water solubility were performed at 20 (±0.5) °C.	Acceptable Moderately soluble in double distilled water, acetate buffer and borate buffer. The HPLC method for the quantification of the concentration of the metabolite was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR CA Volume 3 Section B.5 (Study no. VP 031/2015)	Y	[see 2015/1139994 Wilbrand S. 2015 c]
	EEC A.6 OECD 105 HPLC method for the determination of Reg.No. 6003432	Reg.No. 6003432, L87-32-1: 97.0 %	<u>M750F007 (Reg.No. 6003432): Flask method (solubility > 0.01 g/L)</u> Double Distilled Water 72.7 (± 11.4) mg/L, pH 6.4 Acetate Buffer 73.4 (± 1.2) mg/L, pH 4.3 Borate Buffer 71.8 (± 2.5) mg/L, pH 8.9 Note: pH values reflect average values of the saturated solutions. Determinations of water	Acceptable Moderately soluble in double distilled water, acetate buffer and borate buffer. The HPLC method for the quantification of the	Y	[see 2015/1139997 Wilbrand S. 2015 d]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	(Study no. VP 032/2015)		solubility were performed at 20 (±0.5) °C.	concentration of the metabolite was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR CA Volume 3 Section B.5 (Study no. VP 032/2015)		
	EEC A.6 OECD 105 HPLC method for the determination of Reg.No. 6010286 (Study no. VP 030/2015)	Reg.No. 6010286, L85-94: 96.5 %	<u>M750F008 (Reg.No. 6010286): Column elution method (solubility < 0.01 g/L)</u> Double Distilled Water 1.96 (± 0.10) mg/L, pH 6.4 Acetate Buffer 2.43 (± 0.21) mg/L, pH 4.4 Borate Buffer 3.67 (± 0.34) mg/L, pH 9.1 Note: pH values reflect average values of the saturated solutions. Determinations of water solubility were performed at 20 (±0.5) °C.	Acceptable Slightly soluble in double distilled water, acetate buffer and borate buffer The HPLC method for the quantification of the concentration of the metabolite was found to be fit for purpose but not fully validated in accordance with SANCO/3029/99 rev.4 in the DAR CA Volume 3 Section B.5 (Study no. VP 030/2015)	Y	[see 2015/1139998 Wilbrand S. 2015 e]
Partition coefficient n-octanol/water **log Pow of the metabolites** **M750F003 (Reg.No. 5924326)** **M750F005 (Reg.No. 6003433)** **M750F006 (Reg.No. 5863469)** **M750F007 (Reg.No. 6003432)** **M750F008 (Reg.No. 6010286)**	EEC A.8 (HPLC method) OECD 117	Reg.No. 5924326, L84-250: 99.6 %	<u>M750F003 (Reg.No. 5924326):</u> Water P_{OW} 2.59, log P_{OW} 0.41, pH 6.8 Acetate Buffer P_{OW} 2.35, log P_{OW} 0.37, pH 4.4 Borate Buffer P_{OW} < 1, log P_{OW} < 0, pH 9.0 Note: determinations of log P_{OW} values were performed at 25 (±1) °C using the HPLC method.	Acceptable According to EEC A.8, the HPLC method is applicable within the range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method).	Y	[see 2015/1139989 Wilbrand S. 2015 a] [see 2015/1252305 Wilbrand S. 2016 a] see 2016/1030230 Wilbrand S. 2016 b]
		Reg.No. 6003433, L87-34: 99.4 %	<u>M750F005 (Reg.No. 6003433):</u> Water P_{OW} 48.98, log P_{OW} 1.69, pH 6.8 Acetate Buffer P_{OW} 25.29, log P_{OW} 1.41, pH 4.4	Acceptable According to EEC A.8, the HPLC method is applicable within the	Y	[see 2015/1139993 Wilbrand S. 2015 b]

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			Borate Buffer P_{OW} 9.22, log P_{OW} 0.96, pH 9.0 Note: determinations of log P_{OW} values were performed at 25 (±1) °C using the HPLC method.	range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method).		
		Reg.No. 5863469, L87-30: 98.9 %	<u>M750F006 (Reg.No. 5863469):</u> Water P_{OW} 538.1, log P_{OW} 2.73, pH 6.8 Acetate Buffer P_{OW} 305.9, log P_{OW} 2.49, pH 4.3 Borate Buffer P_{OW} 352.9, log P_{OW} 2.55, pH 9.0 Note: determinations of log P_{OW} values were performed at 25 (±1) °C using the HPLC method.	Acceptable According to EEC A.8, the HPLC method is applicable within the range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method).	Y	[see 2015/1139994 Wilbrand S. 2015 c]
		Reg.No. 6003432, L87-32-1: 97.0 %	<u>M750F007 (Reg.No. 6003432):</u> Water P_{OW} 7.91, log P_{OW} 0.90, pH 6.8 Acetate Buffer P_{OW} 7.82, log P_{OW} 0.89, pH 4.4 Borate Buffer P_{OW} < 1, log P_{OW} < 0, pH 9.0 Note: determinations of log P_{OW} values were performed at 25 (±1) °C using the HPLC method.	Acceptable According to EEC A.8, the HPLC method is applicable within the range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method).	Y	[see 2015/1139997 Wilbrand S. 2015 d]
		Reg.No. 6010286, L85-94: 96.5 %	<u>M750F008 (Reg.No. 6010286):</u> Water P_{OW} 57.36, log P_{OW} 1.76, pH 6.8 Acetate Buffer P_{OW} 31.35, log P_{OW} 1.49, pH 4.4 Borate Buffer P_{OW} < 1, log P_{OW} < 0, pH 9.0 Note: determinations of log P_{OW} values were performed at 25 (±1) °C using the HPLC method.	Acceptable According to EEC A.8, the HPLC method is applicable within the range log P_{ow} 0 to 6. Hence acceptable that OECD 117 (HPLC method) has been used here rather than OECD 107 (shake flask method).	Y	[see 2015/1139998 Wilbrand S. 2015 e]
Dissociation constant of the	OECD 112	Reg.No. 5924326,	<u>M750F003 (Reg.No. 5924326):</u> pKa = 8.7 (± 0.1) at 20°C	Acceptable	Y	[see 2015/1139989

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
metabolites **M750F003 (Reg.No. 5924326)** **M750F005 (Reg.No. 6003433)** **M750F006 (Reg.No. 5863469)** **M750F007 (Reg.No. 6003432)** **M750F008 (Reg.No. 6010286)**		L84-250: 99.6 %	pKa = 8.74 (± 0.05) at 30°C			Wilbrand S. 2015 a] [see 2015/1252305 Wilbrand S. 2016 a] see 2016/1030230 Wilbrand S. 2016 b]
		Reg.No. 6003433, L87-34: 99.4 %	M750F005 (Reg.No. 6003433): pKa = 9.84 (± 0.05) at 20°C pKa = 9.51 (± 0.07) at 30°C	Acceptable	Y	[see 2015/1139993 Wilbrand S. 2015 b]
		Reg.No. 5863469, L87-30: 98.9 %	M750F006 (Reg.No. 5863469): No dissociation constant found in aqueous solution for 2 < pH < 12. Reg.No. 5863469 contains a lactone structure which might be hydrolyzed under basic conditions by ring-opening. The different UV/Vis spectra in the range above pH 10 are caused by this hydrolysis product.	Acceptable	Y	[see 2015/1139994 Wilbrand S. 2015 c]
		Reg.No. 6003432, L87-32-1: 97.0 %	M750F007 (Reg.No. 6003432): pKa = 9.5 (± 0.1) at 20°C pKa = 9.20 (± 0.14) at 30°C	Acceptable	Y	[see 2015/1139997 Wilbrand S. 2015 d]
		Reg.No. 6010286, L85-94: 96.5 %	M750F008 (Reg.No. 6010286): pKa = 9.09 (± 0.15) at 20°C pKa = 9.10 (± 0.11) at 30°C	Acceptable	Y	[see 2015/1139998 Wilbrand S. 2015 e]

Summary of physical and chemical properties – active substance

The pure active substance BAS 750 F is white, odourless, crystalline powder; as technical grade active substance it is an off-white solid with a moderate thiolic odour. Its melting point is 126 °C and decomposes at approximately 300 °C. It is very slightly – moderately volatile with a vapour pressure of 3.2×10^{-6} Pa at 20 °C and 6.5×10^{-6} at 25 °C and a Henry's Law constant of 1.6×10^{-3}. It is possible that photolytic degradation may occur due to shoulder peaks in its UV/VIS spectrum > 290 nm. Its structure is confirmed by IR, NMR and MS. It is slightly soluble in water, buffer solutions and xylene; moderately soluble in acetone, ethyl acetate, methanol, 1,2-dichloroethane and acetonitrile; and very slightly soluble in n-heptane. The log P_{OW} is 3.4 at pH 7 and has a pKa (calculated) of 3.0. It is not classified as flammable, self-heating, explosive or oxidising in accordance with the CLP regulation.

B.2.15. REFERENCES RELIED ON

BAS 750 F

The following databases were searched:

REAXYS	- Organic compounds, formerly Beilstein	1771 – to present
GESTIS	- Database on hazardous substances of the German Social Accident Insurance	current information
PESTICIDE MANUAL	- 15. Edition, Vers. 5.2 2011/2012	current information
EBSCO EXPUB System with HSDB		current information

Search criteria :

- BAS 750 F, synonyms and CAS numbers were used

A two-step process for selection of relevant scientific peer-reviewed open literature was undertaken:

First Selection step for relevance based on summary records (e.g. titles, abstracts, index terms, keywords)

- Obviously irrelevant records were tagged as "Ballast" and not further processed.
- Records which appeared to be relevant and those of unclear relevance were tagged for further evaluation ("Hits")

Second Detailed Assessment for records requiring further information.
"Hits" were reviewed based on the **title and the abstract** with regard to relevance for the regulatory endpoints. Those records which were clearly not assignable to any regulatory endpoint were categorised as **"no relevant endpoint"**. All remaining records were assessed in detail based on the **complete report** and separated into relevant and non-relevant reports.

Criteria to assign records as **"evaluated - not-relevant"** were:

- Records which did not provide any new relevant data or information
- Records which were not assignable to the substance of interest
- Secondary literature linking to primary literature already discussed under relevant records
- Records with limited reliability of grade 3 or 4 based on the 'Klimisch' scoring system.

Any remaining records were assigned to the category **"used for dossier"**.

1 record relating to BAS 750 F was identified under a consideration of physical and chemical data.

The 1 record relating to BAS 750 F was assessed further and considered not to be relevant to physical and chemical data risk assessment, and have therefore not been included in the dossier.

The methodology used in the search, and determination of records as non-relevant is considered acceptable.

TDMs

The following databased were searched:

Agricola		1979 – to present
ANABSTR	- Analytical Abstracts	1980 – to present
BIOSIS		1926 – to present
CABA	- CAB Abstracts	1973 – to present
CAPLUS	- Chemical Abstracts Plus	1907 – to present
EMBASE		1947 – to present
MEDLINE		1946 – to present
PQScitech		1962 – to present
TOXCENTER		1907 – to present
GEOREF		1669 – to present
FROSTI		1972 – to present
FSTA		1969 – to present
ESBIOBASE		1994 – to present
SCISEARCH		1974 – to present

PASCAL 1977 – to present
CROPB
CROPU
HCHEMLIST

Search criteria:
- 1,2,4-triazole, triazole lactic acid, triazole acetic acid and triazole alanine, synonyms and CAS numbers were used
- Suitable terms relating to product chemistry were used.

The process for selection of relevant scientific peer-reviewed open literature was undertaken as outlined below:
1. A very broad search was conducted for each section of the dossier
2. Duplicate titles were automatically removed
3. A rapid assessment of the titles was conducted to remove any obviously irrelevant titles
4. A further rapid assessment was conducted using abstracts and any clearly irrelevant titles were removed
5. A detailed assessment of the full-text documents for the remaining titles was conducted using the criteria (based on the relevant annex points in the dossier) developed for study relevance.
6. Any relevant papers were highlighted and assessed for reliability.

57 records relating to TDMs were identified under a consideration of product chemistry. All records were considered not to be relevant to the product chemistry risk assessment, and have therefore not been included in the dossier.

Data Point	**Author(s)**	**Year**	**Title Company Report No. Source (where different from company) GLP or GEP status Published or not**	**Vertebrate study Y/N**	**Data protection claimed Y/N**	**Justification if data protection is claimed**	**Owner**	**Previous evaluation**
KCA 2.1/1 KCA 2.2/1 KCA 2.3/1	Kroehl T.	2014 a	Physical properties of Reg.No. 5834378 - Pure active ingredient (PAI) 2014/1117052 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.1/2	Kroehl T.	2014 b	Physical and chemical properties of BAS 750 F (Reg.No. 5834378) technical active ingredient TC -	No	Yes	Data for first Approval	BASF	N.A.

			Accelerated storage stability up to 2 weeks at 54°C 2014/1117053 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished					
KCA 2.2/2	Kroehl T.	2014 c	Henry s law constant for BAS 750 F (Reg.No. 5834378) 2014/1173597 BASF SE, Limburgerhof, Germany Fed.Rep. no Unpublished	No	No	Not applicable	BASF	N.A.
KCA 2.3/2	Kroehl T.	2014 b	Physical and chemical properties of BAS 750 F (Reg.No. 5834378) technical active ingredient TC - Accelerated storage stability up to 2 weeks at 54°C 2014/1117053 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.4/1	Kroehl T. Behnken H.	2014 a	Mass, NMR, IR and UV/Vis spectra of BASF	No	Yes	Data for first Approval	BASF	N.A.

			750 F (Reg.No. 5834378) 2014/1173598 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished					
KCA 2.4/2	Kroehl T.	2015 a	Supplement to study 432182_1 - Mass, NMR, IR and UV/Vis spectra of BAS 750 F (Reg.No. 5834378) 2015/1183750 BASF SE, Limburgerhof, Germany Fed.Rep. no Unpublished	No	No	Not applicable	BASF	N.A.
KCA 2.4/3	Kroehl T.	2016 a	Supplement No. 2 to study 432182_1 - Mass, NMR, IR and UV/Vis spectra of BAS 750 F (Reg.No. 5834378) BASF SE, Limburgerhof, Germany Fed.Rep. 2016/1203119 no Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.5/1	Wilbrand S.	2013 a	Determination of the solubility in distilled water and in buffer solutions at pH 4 and pH 7 (Column Elution Method) of Reg.No.	No	Yes	Data for first Approval	BASF	N.A.

			5834378 2013/1397136 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished					
KCA 2.5/2	Kroehl T.	2016 b	Supplement to study 432184_1 - Determination of the solubility in distilled water and in buffer solutions at pH 4 and pH 7 (Column Elution Method) of Reg.No.: 5834378 BASF SE, Limburgerhof, Germany Fed.Rep. 2016/1203120 no Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.6/1	Wilbrand S.	2013 b	Determination of the solubility in organic solvents of Reg.No. 5834378 2013/1391669 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.7/1	Wilbrand S.	2013 c	Determination of the partition coefficient 1-octanol/water (HPLC method) of Reg.No. 5834378 2013/1382370	No	Yes	Data for first Approval	BASF	N.A.

			Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished					
KCA 2.8/1	Wilbrand S.	2013 d	Determination of the dissociation constant of Reg.No. 5834378 in water according to OECD guideline 112 2013/1397719 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.9/1 KCA 2.10/1 KCA 2.11/1 KCA 2.13/1	Moeller M.	2014 a	BAS 750 F - Determination of physico-chemical properties according to Directive 94/37/EC (Regulation (EC) No. 440/2008) 2014/1109962 consilab Gesellschaft fuer Anlagensicherheit mbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/1	Daum A.	2015 a	Vapour pressure of Reg.No. 5924326 (M750F003)	No	Yes	Data for first Approval	BASF	N.A.

			2015/1205970 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished					
KCA 2.14/2	Daum A.	2015 b	Vapour pressure of Reg.No. 6003433 (M750F005) 2015/1205971 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/3	Daum A.	2015 c	Vapour pressure of Reg.No. 5863469 (M750F006) 2015/1205972 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/4	Daum A.	2015 d	Vapour pressure of Reg.No. 6003432 (M750F007) 2015/1205973 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.

KCA 2.14/5	Daum A.	2015 e	Vapour pressure of Reg.No. 6010286 (M750F008) 2015/1205976 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/6	Wilbrand S.	2015 a	Reg.No. 5924326: Solubility in water (Flask method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water 2015/1139989 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/7	Wilbrand S.	2016 a	Amendment No. 1 - Reg.No. 5924326: Solubility in water (Flask method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water	No	Yes	Data for first Approval	BASF	N.A.

			2015/1252305 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished					
KCA 2.14/8	Wilbrand S.	2016 b	Report amendment No. 2 to final report - Reg.No. 5924326: Solubility in water (Flask method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water (Original No. 2 of 2) 2016/1030230 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/9	Wilbrand S.	2015 b	Reg.No. 6003433: Solubility in water (Column Elution Method) (double distilled water, ph 4, ph 9), partition coefficient 1-Octanol/Water (distilled water, ph 4, ph 9) and dissociation constant in water (original No. 1 of 2)	No	Yes	Data for first Approval	BASF	N.A.

			2015/1139993 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished					
KCA 2.14/10	Wilbrand S.	2015 c	Solubility in water (column elution method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water (original no. 2 of 2) 2015/1139994 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.
KCA 2.14/11	Wilbrand S.	2015 d	Solubility in water (flask method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water (original no. 2 of 2) 2015/1139997 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep.	No	Yes	Data for first Approval	BASF	N.A.

			yes Unpublished					
KCA 2.14/12	Wilbrand S.	2015 e	Reg.No. 6010286: Solubility in water (column elution method) (double distilled water, pH 4, pH 9), partition coefficient 1-octanol/water (distilled water, pH 4, pH 9) and dissociation constant in water (Original No. 2 of 2) 2015/1139998 Allessa GmbH, Frankfurt/Main, Germany Fed.Rep. yes Unpublished	No	Yes	Data for first Approval	BASF	N.A.