Datenbank-Scripte zum Tabellen erstellen

/\*\*\*\*\*\* Object: Table [dbo].[GemesseneStandards] Script Date: 9/29/2022 7:30:45 PM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[GemesseneStandards](

[CAS] [nvarchar](50) NOT NULL,

[Type] [nvarchar](50) NOT NULL,

[RILib] [nvarchar](50) NOT NULL,

[Name] [nvarchar](1000) NOT NULL,

[Remark] [nvarchar](1000) NULL

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[Säule\_BW] Script Date: 9/30/2022 10:15:46 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[Säule\_BW](

[CAS] [nvarchar](50) NULL,

[SysName] [nvarchar](50) NULL,

[Type] [nvarchar](50) NOT NULL,

[Name] [nvarchar](500) NOT NULL

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tb\_bwb\_stoffe] Script Date: 9/30/2022 10:18:24 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tb\_bwb\_stoffe](

[ID\_BWBstoffe] [int] IDENTITY(1,1) NOT NULL,

[IKey\_CAS\_name] [nvarchar](50) NOT NULL,

[BWBname] [nvarchar](max) NOT NULL,

[IUPACname] [nvarchar](max) NOT NULL,

[Formel] [nvarchar](max) NULL,

[MW] [float] NULL,

[SummeVerwendung] [text] NULL,

[Import\_Date] [datetime] NOT NULL,

CONSTRAINT [PK\_tb\_bwb\_stoffe] PRIMARY KEY CLUSTERED

(

[IKey\_CAS\_name] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY] TEXTIMAGE\_ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tb\_cas\_ikey] Script Date: 9/30/2022 10:24:13 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tb\_cas\_ikey](

[ID\_cas] [int] IDENTITY(1,1) NOT NULL,

[Zeile] [int] NOT NULL,

[CAS\_NIST\_name] [nvarchar](50) NOT NULL,

[InChiKey] [nvarchar](50) NULL,

[Woher] [nchar](10) NULL,

[EC\_No] [nvarchar](50) NULL,

[Norman\_SusDat\_ID] [nchar](10) NULL,

[Import\_Date] [datetime] NOT NULL,

CONSTRAINT [PK\_tb\_cas\_ikey] PRIMARY KEY CLUSTERED

(

[Zeile] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tb\_UA\_stoffe] Script Date: 9/30/2022 10:26:07 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tb\_UA\_stoffe](

[ID\_UAstoffe] [int] IDENTITY(1,1) NOT NULL,

[Ikey\_GC\_name] [nvarchar](50) NOT NULL,

[UAname] [nvarchar](150) NOT NULL,

[BPMZ\_UALib] [float] NOT NULL,

[RI\_UALib] [float] NOT NULL,

[Import\_Date] [datetime] NOT NULL,

CONSTRAINT [PK\_tb\_UA\_stoffe] PRIMARY KEY CLUSTERED

(

[Ikey\_GC\_name] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tbBWZuordg] Script Date: 9/30/2022 10:27:11 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tbBWZuordg](

[PKenng] [nvarchar](50) NOT NULL,

[BWZuordg] [nvarchar](50) NOT NULL,

[Alkane\_Zuordg] [nvarchar](50) NULL,

[File\_mess] [nvarchar](50) NULL,

[Acq\_Date\_Time] [nvarchar](50) NULL,

[Import\_Date] [datetime] NOT NULL,

CONSTRAINT [PK\_tbBWZuordg] PRIMARY KEY CLUSTERED

(

[PKenng] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tbLInfos] Script Date: 9/30/2022 10:28:23 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tbLInfos](

[ID\_LInfos] [int] IDENTITY(1,1) NOT NULL,

[LimsNr] [nvarchar](50) NOT NULL,

[ProbenArt] [nvarchar](50) NOT NULL,

[Ort\_kurz] [nvarchar](50) NOT NULL,

[Entnahmedatum] [nvarchar](50) NOT NULL,

[Import\_Date] [datetime] NOT NULL,

CONSTRAINT [PK\_E3\_Lims\_Info] PRIMARY KEY CLUSTERED

(

[LimsNr] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tbPeaks] Script Date: 9/30/2022 10:29:30 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tbPeaks](

[ID\_Peak] [int] IDENTITY(1,1) NOT NULL,

[RTmess] [float] NOT NULL,

[BP\_MZ] [float] NOT NULL,

[CAS] [nvarchar](50) NULL,

[LibRI] [float] NULL,

[RImess] [float] NOT NULL,

[MF] [float] NOT NULL,

[SName] [nvarchar](150) NOT NULL,

[Formula] [nvarchar](50) NULL,

[LibFile] [nvarchar](50) NOT NULL,

[AreaP] [float] NOT NULL,

[AreaBP] [float] NOT NULL,

[Type] [nvarchar](50) NOT NULL,

[PKenng] [nvarchar](50) NOT NULL,

[Import\_Date] [datetime] NULL,

[RTkorr] [float] NULL,

[RIkorr] [int] NULL,

[BPMZ\_RT] [nvarchar](50) NULL,

[BPMZ\_RI] [nvarchar](50) NULL,

[Peak\_minus\_BW] [float] NULL,

[AreaBW] [float] NULL,

[Kategorie] [int] NULL,

[Name\_BPMZ\_RI] [nvarchar](100) NULL,

[AreaPercent] [int] NULL,

CONSTRAINT [PK\_tbPeaks] PRIMARY KEY CLUSTERED

(

[ID\_Peak] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

/\*\*\*\*\*\* Object: Table [dbo].[tbPInfos] Script Date: 9/30/2022 10:30:36 AM \*\*\*\*\*\*/

SET ANSI\_NULLS ON

GO

SET QUOTED\_IDENTIFIER ON

GO

CREATE TABLE [dbo].[tbPInfos](

[ID\_PInfos] [int] IDENTITY(1,1) NOT NULL,

[PKenng] [nvarchar](50) NOT NULL,

[Thema] [nvarchar](50) NULL,

[LM] [nvarchar](50) NULL,

[Vorbereitung\_Meth] [nvarchar](50) NULL,

[RT\_IS\_Pr] [float] NOT NULL,

[RI\_IS\_Pr] [float] NOT NULL,

[IS\_AreaP] [float] NOT NULL,

[IS\_AreaBP] [float] NOT NULL,

[V\_Extraktion\_mL] [float] NOT NULL,

[Verdg\_im\_Vial] [float] NOT NULL,

[IS\_Volumen\_ml] [float] NOT NULL,

[InjektionsVolumen\_ml] [float] NOT NULL,

[Import\_Date] [datetime] NOT NULL,

[BWabgezogen] [bit] NOT NULL,

CONSTRAINT [PK\_tbPInfos] PRIMARY KEY CLUSTERED

(

[PKenng] ASC

)WITH (PAD\_INDEX = OFF, STATISTICS\_NORECOMPUTE = OFF, IGNORE\_DUP\_KEY = OFF, ALLOW\_ROW\_LOCKS = ON, ALLOW\_PAGE\_LOCKS = ON, OPTIMIZE\_FOR\_SEQUENTIAL\_KEY = OFF) ON [PRIMARY]

) ON [PRIMARY]

GO

ALTER TABLE [dbo].[tbPInfos] ADD CONSTRAINT [DF\_tbPInfos\_BWabgezogen] DEFAULT ((0)) FOR [BWabgezogen]

GO

insert into dbo.GemesseneStandards

(CAS, Type, RILib, Name, Remark)

values

('1024-57-3','x','2015','Heptachlor epoxide','CKW std'),

('309-00-2','x','1955','Aldrin','CKW std'),

('33213-65-9','x','2236','beta Endosulfan','CKW std'),

('50-29-3','x','2334','p,p-DDT','CKW std'),

('60-57-1','x','2167','Dieldrin','CKW std'),

('72-20-8','x','2211','Endrin','CKW std'),

('72-54-8','x','2293.3036','p,p DDD','CKW std'),

('72-55-9','x','2169','p,p-DDE','CKW std'),

('76-44-8','x','1887','Heptachlor','CKW std'),

('789-02-6','x','2270','o,p-DDT','CKW std'),

('959-98-8','x','2114','alpha Endosulfan','CKW std'),

('5324-68-5','IS','1706.119','alpha HCH d6 (IS)','CKW std IS'),

('319-84-6','x','1713.364','alpha-1,2,3,4,5,6-Hexachlorocyclohexane','CKW, Std'),

('319-85-7','x','1765.4259','beta-Hexachlorocyclohexane','CKW, Std'),

('319-86-8','x','1825.0956','delta-Hexachlorocyclohexane','CKW, Std'),

('58-89-9','x','1777.0485','Lindane','CKW, Std'),

('1486-01-7','IS','1375','ISTD\_BIPHENYL-D10','IS scan'),

('112-40-3','x','1200','Dodecane','KW std'),

('112-95-8','x','2000','Eicosane','KW std'),

('124-18-5','x','1000','Decane','KW std'),

('544-76-3','x','1600','Hexadecane','KW std'),

('593-45-3','x','1800','Octadecane','KW std'),

('629-59-4','x','1400','Tetradecane','KW std'),

('629-97-0','x','2200','Docosane','KW std'),

('630-01-3','x','2600','Hexacosane','KW std'),

('630-02-4','x','2800','Octacosane','KW std'),

('646-31-1','x','2400','Tetracosane','KW std'),

('100-41-4','x','855','Ethylbenzene','LHKW, Std'),

('106-42-3','x','865','1,4-Dimethylbenzene','LHKW, Std'),

('106-46-7','x','1021','1,4-Dichlorobenzene','LHKW, Std'),

('108-38-3','x','866','1,3-Dimethylbenzene','LHKW, Std'),

('108-90-7','x','849','Chlorobenzene','LHKW, Std'),

('127-18-4','x','815','Tetrachloroethene','LHKW, Std'),

('541-73-1','x','1012','1,3-Dichlorobenzene','LHKW, Std'),

('75-25-2','x','892','Tribromomethane','LHKW, Std'),

('95-47-6','x','888','1,2-Dimethylbenzene','LHKW, Std'),

('95-50-1','x','1043','1,2-Dichlorobenzene','LHKW, Std'),

('98-82-8','x','922','Cumen','LHKW, Std'),

('120-12-7','x','1804.6199','Anthracene','PAK, Std'),

('129-00-0','x','2140.2127','Pyrene','PAK, Std'),

('1520-96-3','IS','2917.8527','Perylene-D12','PAK, Std'),

('191-24-2','x','3361.7307','Benzo[ghi]perylene','PAK, Std'),

('193-39-5','x','3266.7235','Indeno[1,2,3-cd]pyrene','PAK, Std'),

('205-99-2','x','2811.8142','Benzo[b]fluoranthene               P1191','PAK, Std'),

('206-44-0','x','2084.8829','Fluoranthene','PAK, Std'),

('207-08-9','x','2818.2696','Benzo[k]fluoranthene','PAK, Std'),

('208-96-8','x','1458.204','Acenaphthylene','PAK, Std'),

('218-01-9','x','2497.2984','Chrysene','PAK, Std'),

('50-32-8','x','2901.1916','Benzo[a]pyrene','PAK, Std'),

('53-70-3','x','3280.4027','Dibenz[a,h]anthracene','PAK, Std'),

('56-55-3','x','2485.8323','Benz[a]anthracene','PAK, Std'),

('83-32-9','x','1495.0173','Acenaphthene','PAK, Std'),

('85-01-8','x','1794.7289','Phenanthrene','PAK, Std'),

('86-73-7','x','1592.6817','Fluorene','PAK, Std'),

('91-20-3','x','1185.3303','Naphthalene','PAK, Std'),

('1718-53-2','IS','2479.5569','Benz[a]anthracene-D12','PAK, Std'),

('81103-79-9','IS','1587.5237','Fluorene-D10','PAK, Std'),

('117-81-7','x','2558.7459','Bis(2-ethylhexyl) phthalate','PHTH std'),

('117-84-0','x','2745.9612','Di-n-octyl phthalate','PHTH std'),

('131-11-3','x','1454','Dimethyl phthalate','PHTH std'),

('84-66-2','x','1598','Diethyl phthalate','PHTH std'),

('84-74-2','x','1973','Dibutyl phthalate','PHTH std'),

('84-76-4','x','2896.3074','Dinonyl phthalate','PHTH std'),

('85-68-7','x','2336','Benzyl butyl phthalate','PHTH std'),

('70-55-3','x','1673','p-Toluenesulfamide','pTSA-Std'),

('137-58-6','x','1912','Lidocaine','std Arzeneistoff: örtliches Beteubungsmittel'),

('298-46-4','x','2314','Carbamazepine','std, Antiepileptika'),

('115-86-6','x','2420.4087','Triphenyl phosphate','Std, LC'),

('115-96-8','x','1777.3671','Tri(2-chloroethyl) phosphate','Std, LC'),

('126-73-8','x','1658.5442','Tributyl phosphate','Std, LC'),

('134-62-3','x','1592.1183','Diethyltoluamide','Std, LC'),

('13674-84-5','x','1814','Tris(2-chloroisopropyl)phosphate','Std, LC'),

('479-92-5','x','1939','Propyphenazone','Std, LC'),

('54-11-5','x','1361.8102','Nicotine','Std, LC'),

('95-14-7','x','1469','1,2,3-Benzotriazole','Std, LC'),

('7421-93-4','x','2261','1,2,4-Methenocyclopenta[cd]pentalene-5-carboxaldehyde, 2,2a,3,3,4,7-hexachlorodecahydro-, (1.alpha.,2.beta.,2a.beta.,4.beta.,4a.beta.,5.beta.,6a.beta.,6b.beta.,7R\*)-','CKW, Std'),

('101-80-4','x','2140','4,4-Oxydianiline','Std'),

('120-75-2','x','1281','2-Methyl-Benzothiazole','Std'),

('128-37-0','x','1513','Butylated Hydroxytoluene','Std'),

('144-83-2 ','x','2378','Sulfapyridine','Std'),

('3470-98-2','x','1218','2-Pyrrolidinone, 1-butyl-','std'),

('54143-55-4 ','x','2231','Flecainide','Std'),

('59729-33-8','x','2407','Citalopram','std'),

('78-40-0','x','1137','Triethyl phosphate','std'),

('84057-84-1 ','x','2547',' Lamotrigine','Std'),

('934-34-9','x','1630','2(3H)-Benzothiazolone','std'),

('1031-07-8','x','2329','Endosulfan sulfate','CKW std'),

('15067-26-2','IS','1475','Acenaphthene-d10','PAK, Std'),

('98-86-2','x','1066','Acetophenone','std')

insert into dbo.Säule\_BW

(CAS, SysName, Type, Name)

values

('1000163-31-6', NULL, 'Säule', 'Silane, (3,3-dimethylbut-2-yloxy)-(phenyl)-'),

('1000363-04-7', NULL, 'Säule', 'Silane, diethylbutoxy(2-ethylhexyloxy)-'),

('1000363-09-9', NULL, 'Säule', 'Silane, diethyl(2-methylbutoxy)pentyloxy-'),

('1000416-18-6', NULL, 'Säule', 'Silane, methyldiethoxyisopropoxy-'),

('1000416-90-5', NULL, 'Säule', 'Silane, methylvinyl(2,4-dimethylpent-3-yloxy)ethoxy-'),

('1068-69-5', NULL, 'Säule', 'Silane, methylidynetris[trimethyl-'),

('107-50-6', NULL, 'Säule', 'Cycloheptasiloxane, tetradecamethyl-'),

('14920-92-4', NULL, 'Säule', 'Pentamethylphenyldisiloxane'),

('1825-61-2', NULL, 'Säule', 'Silane, methoxytrimethyl-'),

('18919-94-3', NULL, 'Säule', 'Tetracosamethylcyclododecasiloxane'),

('2031-67-6', NULL, 'Säule', 'Silane, triethoxymethyl-'),

('540-97-6', NULL, 'Säule', 'Dodecamethylcyclohexasiloxane'),

('541-01-5', NULL, 'Säule', 'Hexadecamethylheptasiloxane'),

('541-02-6', NULL, 'Säule', 'Decamethylcyclopentasiloxane'),

('541-05-9', NULL, 'Säule', 'Hexamethylcyclotrisiloxane'),

('556-67-2', NULL, 'Säule', 'Octamethylcyclotetrasiloxane'),

('556-68-3', NULL, 'Säule', 'Hexadecamethylcyclooctasiloxane'),

('556-71-8', NULL, 'Säule', 'Octadecamethylcyclononasiloxane'),

('74810-38-1', NULL, 'Säule', 'Silane, (iodomethyl)dimethylpropyl-'),

(NULL, 'GC\_BPMZ\_327\_RI\_1891', 'Säule', 'GC\_BPMZ\_327\_RI\_1891'),

(NULL, 'GC\_BPMZ\_281\_RI\_1009', 'Säule', 'GC\_BPMZ\_281\_RI\_1009'),

(NULL, 'GC\_BPMZ\_147\_RI\_2285', 'Säule', 'GC\_BPMZ\_147\_RI\_2285'),