



**Thermo Scientific**  
Technical Resources Document

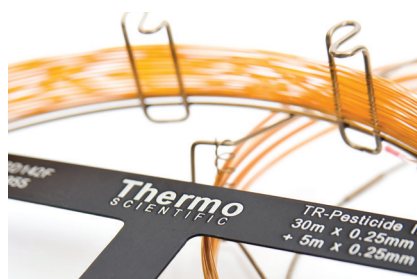
# GC Columns and Accessories

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# GC Column Selection

When selecting a GC column for your analysis, it can often be difficult to choose the most appropriate column because of the wide range of options. However, the choice can be simplified by considering a number of questions about the planned separation. This section provides useful information to help you determine the most suitable column for your analysis.



## Column Selection for Existing or Regulated Methods

This section provides a number of tools to aid in selecting the most appropriate Thermo Scientific GC column. The Thermo Scientific GC column phase table lists details for the wide array of phases offered in the TraceGOLD, TRACE and TracePLOT GC column ranges. The GC column selection by manufacturer table provides a quick cross reference for Thermo Scientific columns to other GC column manufacturers. If you are following an ASTM, NIOSH or US EPA method, please refer to the column selection by method tables for the best Thermo Scientific product.

## Method Development Considerations

When first developing a method, you should consider these column characteristics to determine the best column for the separation:

- Column Phase
- Internal Diameter
- Film Thickness
- Column Length

### A. Column Phase

In GC, the separation of two analytes occurs due to differences in their interaction with the stationary phase, therefore a phase must be chosen that matches the properties of the sample. For example, if the components have different boiling points (greater than 2°C), a non-polar column such as the TG-1MS is recommended. If the products differ primarily in their polarities, then a polar column such as the TG-WaxMS will be ideal.

If you know the particular class of your sample, please refer to the column selection by application for a recommended phase (see page 3-010). Always select the least polar column which will perform the separation.

### B. Internal Diameter

The selection of the internal diameter is often determined by the instrument or detection method. Most modern GC equipment will accommodate most column sizes. With a larger internal diameter, column sample capacity increases, but resolution and sensitivity decrease. Conversely, a smaller ID column can improve resolution and sensitivity, but with the drawback of reduced sample capacity and a greater need for sample preparation. It is a good idea to find a similar application which gives separation of the desired components and use this as a guide.

### C. Film Thickness

Increasing the film thickness increases the sample capacity of the column and slows the elution of the peaks which can help when analyzing volatile compounds. A thicker film also reduces the potential of overloading the column, thus improving the resolution. However, a thicker film can be more sensitive to degradation. The same component will elute at a higher temperature on a thick film when compared to a thin film.

Compounds with high boiling points or those with a high molecular weight should be analyzed using a thin film to improve resolution and avoid unnecessarily long analysis times.

Another factor to consider is the phase ratio ( $\beta$ ) which is calculated using both the internal diameter and film thickness in the following equation:

$$\beta = \frac{\text{Internal diameter } (\mu\text{m})}{4 \times \text{Film thickness } (\mu\text{m})}$$

The phase ratio can be used in two ways:

- To categorize the best dimensions for an application:
  - For volatile samples  $\beta < 100$
  - For general samples  $\beta \sim 250$
  - For high molecular weight samples  $\beta > 400$

- To transfer an analysis from a column of one ID to another without changing the method substantially, choose a column with a similar  $\beta$  value as this will have similar retention properties.

Internal Diameter (mm)	Film Thickness ( $\mu\text{m}$ )					
	0.1	0.25	0.5	1	1.8	3
0.1	250	100	50	25	14	8
0.25	625	250	125	63	35	21
0.32	800	320	160	80	44	27
0.53	1325	530	265	133	74	44

Phase ratio ( $\beta$ ) of common column dimensions

### D. Column Length

A longer column length will provide greater efficiency and resolution, but this is not a linear relationship. Resolution is proportional to the square root of column length, so doubling the column length will increase resolution by approximately 40%. However, increasing the column length will also increase the retention time. Double column length, twice the analysis time. Generally, it is recommended to use the shortest column which will perform the desired separation.

### Additional Considerations

Several generalizations regarding GC columns exist that you might rely on when in doubt. First, 95% of all GC columns used are either TG-1MS, TG-5MS or TG-WaxMS type columns. A good starting column is a 30m x 0.25mm ID, 5% Phenyl column with a 0.25 $\mu\text{m}$  film thickness, such as the TG-5MS. (Part number 26098-1420);

This is a non-polar column, which separates predominately on boiling point, but has some polar characteristics.

*For further assistance in choosing the right column for your separation, please contact our technical support help desk.*  
[www.thermoscientific.com/chromexpert](http://www.thermoscientific.com/chromexpert)

## GC Column Phase Information

Range	Column	Phase	Polarity	Maximum Operating Temperature
TraceGOLD	TG-1MS	100% Methylpolysiloxane	Non-Polar	330°C / 350°C
	TG-XLBMS	Proprietary	Non-Polar	360°C
	TG-5MS	5% Phenyl Methylpolysiloxane	Non-Polar	330°C / 350°C
	TG-SQC	Proprietary	Non-Polar	330°C / 350°C
	TG-5MS AMINE	Base Optimised 5% Phenyl Methylpolysiloxane	Non-Polar	300°C / 315°C
	TG-5SiIMS	Similar to 5% Phenyl Methylpolysiloxane	Non-Polar	330°C / 350°C
	TG-5HT	5% Phenyl Methylpolysiloxane	Non-Polar	380°C / 400°C
	TG-35MS	35% Phenyl Methylpolysiloxane	Mid-Polarity	300°C / 320°C
	TG-35MS AMINE	Base Optimised 35% Phenyl Methylpolysiloxane	Mid-Polarity	220°C
	TG-1301MS	6% Cyanopropylphenyl Methylpolysiloxane	Mid-Polarity	260°C / 280°C
	TG-624	6% Cyanopropylphenyl Methylpolysiloxane	Mid-Polarity	240°C
	TG-624SiIMS	Similar to 6% Cyanopropylphenyl Methylpolysiloxane	Mid-Polarity	320°C
	TG-VRX	Proprietary		260°C
	TG-VMS	Proprietary		260°C
	TG-1701MS	14% Cyanopropylphenyl Methylpolysiloxane	Mid-Polarity	260°C / 280°C
	TG-17MS	50% Phenyl Methylpolysiloxane	Mid-Polarity	300°C / 320°C
	TG-17SiIMS	Similar to 50% Phenyl Methylpolysiloxane	Mid-Polarity	340°C / 360°C
	TG-225MS	50% Cyanopropylmethyl Phenylmethylpolysiloxane	Mid-Polarity	220°C / 240°C
	TG-200MS	Trifluoropropyl Methylpolysiloxane	Mid-Polarity	320°C / 340°C
	TG-WaxMS	Polyethylene Glycol (PEG)	Polar	240°C / 260°C
	TG-WaxMS A	Acid Optimised Polyethylene Glycol (PEG)	Polar	240°C / 250°C
	TG-WaxMS B	Base Optimised Polyethylene Glycol (PEG)	Polar	200°C / 220°C
	TG-OCP I	Proprietary		340°C
	TG-OCP II	Proprietary		340°C
	TG-OPP I	Proprietary		330°C
	TG-OPP II	Proprietary		330°C
	TG-ALC I	Proprietary		260°C
	TG-ALC II	Proprietary		260°C
	TG-Dioxin	Proprietary		340°C
	TG-POLAR	95% Cyanopropyl Phenylpolysiloxane	Polar	275°C
	TG-1MT	100% Methylpolysiloxane	Non-Polar	430°C
	TG-5MT	5% Phenyl Methylpolysiloxane	Non-Polar	430°C
	TG-WaxMT	Polyethylene Glycol (PEG)	Polar	240°C / 260°C



GC Column Phase Information *continued*

Range	Column	Phase	Polarity	Maximum Operating Temperature	
TRACE	TR-1MS	100% Dimethyl Polysiloxane	Non-Polar	340°C / 360°C	
	TR-5	5% Phenyl Methylpolysiloxane	Non-Polar	320°C / 340°C for films ≤ 1.5µm 280°C / 300°C for films > 1.5µm	
	TR-5MS	5% Phenyl Polysilphenylene-siloxane	Non-Polar	360°C / 370°C for films ≤ 1.5µm 350°C / 360°C for films > 1.5µm	
	TR-5HT	5% Phenyl Polycarborane Siloxane	Non-Polar	380°C / 400°C	
	TR-35MS	35% Phenyl Polysilphenylene-siloxane	Mid-Polarity	330°C / 360°C	
	TR-1701	14% Cyanopropylphenyl Polysiloxane	Mid-Polarity	280°C / 300°C	
	TR-50MS	50% Phenyl Polysilphenylene-siloxane	Mid-Polarity	360°C / 370°C	
	TR-225	50% Cyanopropylphenyl Polysiloxane	Mid-Polarity	230°C / 250°C	
	TR-Wax	Polyethylene Glycol (PEG)	Polar	260°C / 280°C for films ≤ 1.0µm 240°C / 260°C for films > 1.0µm	
	TR-WaxMS	Polyethylene Glycol (PEG)	Polar	260°C / 280°C	
	TR-FFAP	TPA Modified Polyethylene Glycol (PEG)	Polar	240°C / 250°C	
	TR-SimDist	100% Dimethyl Polysiloxane	Non-Polar	400°C for films ≤ 1.0µm 370°C for 2.65µm films	
	TR-V1	6% Cyanopropylphenyl Polysiloxane	Mid-Polarity	280°C / 300°C	
	TR-FAME	70% Cyanopropyl Polysilphenylene-siloxane	Polar	250°C / 260°C	
	TR-524	Cyanopropylphenyl Dimethyl Polysiloxane	Mid-Polarity	240°C / 260°C	
	TR-525	Proprietary	Mid-Polarity	340°C / 360°C	
	TR-527	5% Phenyl Polysilphenylene-siloxane	Non-Polar	330°C / 350°C	
	TR-8095	8% Phenyl Polycarborane-siloxane	Mid-Polarity	360°C / 370°C	
	TR-8270	5% Phenyl Polysilphenylene-siloxane	Non-Polar	330°C / 350°C	
	TR-PCB 8MS	8% Phenyl Polysilphenylene-siloxane	Mid-Polarity	330°C / 350°C	
	TR-Dioxin 5MS	5% Phenyl Polysilphenylene-siloxane	Non-Polar	330°C / 350°C	
	TR-Biodiesel (M)	100% Dimethyl Polysiloxane	Non-Polar	300°C / 320°C	
	TR-Biodiesel (F)	Polyethylene Glycol (PEG)	Polar	280°C / 300°C	
	TR-Biodiesel (G)	5% Phenyl Polysilphenylene-siloxane	Non-Polar	380°C / 400°C	
	TR-DoA5	5% Phenyl Methylpolysiloxane	Non-Polar	330°C / 350°C	
	TR-DoA35	35% Phenyl Polysilphenylene-siloxane	Mid-Polarity	330°C / 350°C	
	TR-Pesticide	5% Phenyl Methylpolysiloxane	Non-Polar	330°C / 350°C	
	TR-Pesticide II	Proprietary	Non-Polar	330°C / 350°C	
	TR-Pesticide III	35% Phenyl Methylpolysiloxane	Mid-Polarity	300°C / 320°C	
	TR-Pesticide IV	35% Phenyl Methylpolysiloxane	Mid-Polarity	300°C / 320°C	
	TracePLOT	TG-Bond Alumina (Na <sub>2</sub> SO <sub>4</sub> )	Na <sub>2</sub> SO <sub>4</sub> Deactivated Aluminium Oxide	Non-Polar	200°C
		TG-Bond Alumina (KCl)	KCl Deactivated Aluminium Oxide	Non-Polar	200°C
		TG-Bond Msieve 5A	Molecular Sieve (5A)	Non-Polar	300°C
TG-Bond Q		100% Divinylbenzene	Non-Polar	280°C / 300°C	
TG-Bond Q+		Porous Divinylbenzene Polymer	Mid-Polarity	250°C	
TG-Bond S		Divinylbenzene 4-Vinylpyridine	Mid-Polarity	250°C	
TG-Bond U		Divinylbenzene Ethylene Glycol / Dimethylacrylate	Polar	190°C	

Download a copy of our GC column selector mobile app  
[www.thermoscientific.com/tracegold](http://www.thermoscientific.com/tracegold)

Thermo  
 TR-5MS  
 30m x 0.25mm

## GC Column Selection by Manufacturer

Column	Phase	Manufacturer	Recommended Thermo Scientific Alternative(s)
Capillary	007-1(MS)	Quadrex	TG-1MS
	007-17(MPS-50)	Quadrex	TG-17MS
	007-1701	Quadrex	TG-1701MS
	007-2(MP-5)	Quadrex	TG-5MS
	007-2(MPS-5)	Quadrex	TG-5SiIMS
	007-23	Quadrex	TR-FAME
	007-5MS	Quadrex	TG-5MS
	007-624	Quadrex	TG-624
	007-CW	Quadrex	TG-WaxMS
	AT-5	Alltech	TR-5
	AT50	Alltech	TG-17MS
	AT-5MS	Alltech	TG-5MS
	AT-624	Alltech	TG-624
	AT-Silar	Alltech	TR-FAME
	AT-Wax	Alltech	TR-WaxMS
	BP10	SGE	TG-1701MS
	BP20	SGE	TG-WaxMS
	BP21	SGE	TG-WaxMS A TR-FFAP
	BP225	SGE	TG-225MS
	BP5	SGE	TG-5MS
	BP624	SGE	TG-624 TG-624SiIMS
	BPX1	SGE	TG-1MS TR-SimDist
	BPX5	SGE	TG-5MS
	BPX50	SGE	TG-17MS TG-17SiIMS
	BPX608	SGE	TG-35MS
	BPX70	SGE	TR-FAME
	BPX90	SGE	TG-POLAR
	BPX-Volatiles	SGE	TG-624
	CARBOWAX	Agilent	TR-WaxMS
	CP-1301	Agilent	TG-1301MS
	CP-FFAP CB	Agilent	TG-WaxMS A TR-FFAP
	CP-Select624CB	Agilent	TG-624
	CP-Sil 19CB	Agilent	TG-1701MS
	CP-Sil 5CB MS	Agilent	TG-1MS
	CP-Sil 88	Agilent	TG-5SiIMS
	CP-Sil 8CB	Agilent	TG-5SiIMS
	CP-SimDist	Agilent	TR-SimDist
	CP-Wax 51 (Amines)	Agilent	TG-WaxMS B
	CP-Wax 52CB	Agilent	TG-WaxMS TG-WaxMT
	CP-Wax 58 CB (FFAP)	Agilent	TG-WaxMS A TR-FFAP

GC Column Selection by Manufacturer *continued*

Column	Phase	Manufacturer	Recommended Thermo Scientific Alternative(s)
Capillary	DB-1	Agilent	TG-1MS TR-1MS
	DB-1301	Agilent	TG-1301MS
	DB-17	Agilent	TG-17MS
	DB-1701	Agilent	TG-1701MS
	DB-17ht	Agilent	TG-17MS
	DB-17ms	Agilent	TG-17MS TG-17SiIMS
	DB-1ms	Agilent	TG-1MS TR-1MS
	DB-200	Agilent	TG-200MS
	DB-225	Agilent	TG-225MS
	DB-225ms	Agilent	TG-225MS
	DB-23	Agilent	TR-FAME
	DB-2887	Agilent	TR-SimDist
	DB-35	Agilent	TG-35MS
	DB-35ms	Agilent	TG-35MS
	DB-5	Agilent	TR-5 TG-5MS
	DB-5.625	Agilent	TG-5MS
	DB-5ht	Agilent	TG-5HT TG-5MT
	DB-5ms	Agilent	TG-5MS TG-5SiIMS
	DB-624	Agilent	TG-624 TG-624SiIMS
	DB-ALC1	Agilent	TG-ALC Plus I
	DB-ALC2	Agilent	TG-ALC Plus II
	DB-FFAP	Agilent	TG-WaxMS A TR-FFAP
	DB-HT Sim Dis	Agilent	TR-SimDist
	DB-PETRO	Agilent	TG-1MS
	DB-WAX	Agilent	TG-WaxMS TG-WaxMT
	DB-WAXetr	Agilent	TR-WaxMS TG-WaxMS
	DB-XLB	Agilent	TG-XLBMS
	Elite-1301	PerkinElmer	TG-1301MS
	Elite-17	PerkinElmer	TG-17MS
	Elite-1701	PerkinElmer	TG-1701MS
	Elite-17ms	PerkinElmer	TG-17MS
	Elite-200	PerkinElmer	TG-200MS
	Elite-23	PerkinElmer	TR-FAME
	Elite-35ms	PerkinElmer	TG-35MS
	Elite-5	PerkinElmer	TR-5
	Elite-5ms	Perkin Elmer	TG-5MS
	Elite-5ht	PerkinElmer	TG-5HT
	Elite-624	PerkinElmer	TG-624
	Elite-FFAP	PerkinElmer	TG-WaxMS A TR-FFAP
	Elite-WAX	PerkinElmer	TG-WaxMS
	Elite-WAX ETR	PerkinElmer	TG-WaxMS

Column	Phase	Manufacturer	Recommended Thermo Scientific Alternative(s)
Capillary	HP-1	Agilent	TG-1MS TR-1MS
	HP-17	Agilent	TG-17MS TG-17SiIMS
	HP-1701	Agilent	TG-1701MS
	HP-1MS	Agilent	TG-1MS TG-1MT
	HP20M	Agilent	TG-WaxMS
	HP-23	Agilent	TR-FAME
	HP-35	Agilent	TG-35MS
	HP-35MS	Agilent	TG-35MS
	HP-5	Agilent	TR-5
	HP-50+	Agilent	TG-17MS
	HP-5MS	Agilent	TG-5MS TG-5SiIMS
	HP5-TA	Agilent	TG-5MS
	HP-88	Agilent	TR-FAME
	HP-FFAP	Agilent	TG-WaxMS A TR-FFAP
	HP-INNOWax	Agilent	TG-WaxMS TR-WaxMS
	HP-VOC	Agilent	TG-624 TG-624SiIMS
	HP-Wax	Agilent	TG-WaxMS TR-WaxMS
	HT5	SGE	TG-5HT
	HT8	SGE	TR-PCB 8MS
	MDN-1	Sigma Aldrich	TG-1MS
	MDN-35	Sigma Aldrich	TG-35MS
	MDN-5	Sigma Aldrich	TR-5 TG-5MS
	MDN-5S	Sigma Aldrich	TG-5SiIMS
	Nukol	Sigma Aldrich	TG-WaxMS
	OV-17	Ohio Valley	TG-17MS
	OV-1701	Ohio Valley	TG-1701MS
	OV-5	Ohio Valley	TR-5
	OV-624	Ohio Valley	TG-624
	Petrocol 2887	Sigma Aldrich	TR-SimDist
	Petrocol DH	Sigma Aldrich	TG-1MS
	Petrocol EX2887	Sigma Aldrich	TR-SimDist
	MXT-1	Restek	TG-1MT
	MXT-5	Restek	TG-5MT
	MXT-WAX	Restek	TG-WaxMT
	Rtx-1301	Restek	TG-1301MS
	Rtx-1701	Restek	TG-1701MS
	Rtx-1MS	Restek	TG-1MS
	Rtx-200	Restek	TG-200MS
	Rtx-200MS	Restek	TG-200MS
	Rtx-225	Restek	TG-225MS
	Rtx-2330	Restek	TG-POLAR
	Rtx-2560	Restek	TR-FAME
Rtx-2887	Restek	TR-SimDist	
Rtx-35	Restek	TG-35MS	
Rtx-35 Amine	Restek	TG-35MS AMINE	



GC Column Selection by Manufacturer *continued*

Column	Phase	Manufacturer	Recommended Thermo Scientific Alternative(s)
Capillary	Rtx-35MS	Restek	TG-35MS
	Rtx-5	Restek	TG-5MS TR-5
	Rtx-5 Amine	Restek	TG-5MS AMINE
	Rtx-50	Restek	TG-17MS
	Rtx-5SiIMS	Restek	TG-5SiIMS
	Rtx-624	Restek	TG-624
	Rtx-CLPesticides	Restek	TG-OCP I
	Rtx-CLPesticides2	Restek	TG-OCP II
	Rtx-OPPesticides	Restek	TG-OPP I
	Rtx-OPPesticides2	Restek	TG-OPP II
	Rtx-Dioxin 2	Restek	TG-Dioxin
	Rtx-VMS	Restek	TG-VMS
	Rtx-Volatiles	Restek	TG-624
	Rtx-VRX	Restek	TG-VRX
	Rtx-Wax	Restek	TG-WaxMS
	Rxi-17	Restek	TG-17MS
	Rxi-17SiIMS	Restek	TG-17SiIMS
	Rxi-1ms	Restek	TG-1MS
	Rxi-5HT	Restek	TG-5HT
	Rxi-5MS	Restek	TG-5MS
	Rxi-5SiIMS	Restek	TG-5SiIMS
	Rxi-624SiIMS	Restek	TG-624SiIMS
	Rxi-XLB	Restek	TG-XLBMS
	SE-30	Agilent	TG-1MS
	SE-52	Agilent	TG-5MS
	SE-54	Agilent	TG-5MS
	SolGel-Wax	SGE	TG-WaxMS
	SP-2100	Supelco	TG-1MS
	SP-2250	Supelco	TG-17MS
	SP-2330	Supelco	TR-FAME
	SP-2380	Supelco	TR-FAME
	SPB-1	Supelco	TG-1MS
	SPB-17	Supelco	TG-17MS
	SPB-35	Supelco	TG-35MS
	SPB-5	Supelco	TR-5 TG-5MS
	SPB-50	Supelco	TG-17MS
	SUPELCOWAX-10	Supelco	TG-WaxMS TR-WaxMS
	Stabilwax	Restek	TG-WaxMS
	Stabilwax-DA	Restek	TG-WaxMS A TR-FFAP
	Stabilwax-DB	Restek	TG-WaxMS B
	SUPELCOWAX-10	Supelco	TG-WaxMS
	VF-17ms	Agilent	TG-17MS TG-17SiIMS
	VF-1ms	Agilent	TG-1MS TR-1MS
	VF-200ms	Agilent	TG-200MS
	VF-23ms	Agilent	TR-FAME
	VF-35ms	Agilent	TG-35MS
	VF-5ht	Agilent	TG-5HT
VF-5ms	Agilent	TG-5MS	
VF-Xms	Agilent	TG-XLBMS	

Column	Phase	Manufacturer	Recommended Thermo Scientific Alternative(s)	
Capillary	ZB-1701	Phenomenex	TG-1701MS	
	ZB-1701P	Phenomenex	TG-WaxMS	
	ZB-1HT Inferno	Phenomenex	TR-SimDist	
	ZB-1MS	Phenomenex	TG-1MS	
	ZB-35	Phenomenex	TG-35MS	
	ZB-5	Phenomenex	TR-5	
	ZB-50	Phenomenex	TG-17MS TG-17SiIMS	
	ZB-5HT Inferno	Phenomenex	TG-5HT	
	ZB-5MS	Phenomenex	TG-5MS	
	ZB-5MS Si	Phenomenex	TG-5SiIMS	
	ZB-624	Phenomenex	TG-624 TG-624SiIMS	
	ZB-FFAP	Phenomenex	TG-WaxMS A TR-FFAP	
	ZB-Wax	Phenomenex	TG-WaxMS	
	ZB-Waxplus	Phenomenex	TR-WaxMS	
	PLOT	Alumina-PLOT	Supelco	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )
		AT-Alumina	Alltech	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )
		AT-Molsieve	Alltech	TG-BOND Msieve 5A
AT-Q		Alltech	TG-BOND Q	
CP-AI203/KCl		Agilent	TG-BOND Alumina (KCl)	
CP-AI203/Na <sub>2</sub> SO <sub>4</sub>		Agilent	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )	
CP-Molsieve 5A		Agilent	TG-BOND Msieve 5A	
CP-PoraPLOT Q		Agilent	TG-BOND Q	
CP-PoraPLOT S		Agilent	TG-BOND S	
CP-PoraPLOT U		Agilent	TR-BOND U	
GS-Alumina		Agilent	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )	
GS-Alumina KCl		Agilent	TG-BOND Alumina (KCl)	
GS-Molsieve		Agilent	TG-BOND Msieve 5A	
GS-Q		Agilent	TG-BOND Q+	
HP PLOT M		Agilent	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )	
HP PLOT Molsieve		Agilent	TG-BOND Msieve 5A	
HP PLOT S		Agilent	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )	
HP-UPLLOT		Agilent	TG-BOND U	
PoraBond Q		Agilent	TG-BOND Q	
PoraBond U		Agilent	TG-BOND U	
Molsieve 5A PLOT		Supelco	TG-BOND Msieve 5A	
PLT-5A		Quadrex	TG-BOND Msieve 5A	
Rt-Alumina Bond (KCl)		Restek	TG-BOND Alumina (KCl)	
Rt-Alumina Bond (Na <sub>2</sub> SO <sub>4</sub> )		Restek	TG-BOND Alumina (Na <sub>2</sub> SO <sub>4</sub> )	
Rt-Msieve 5A		Restek	TG-BOND Msieve 5A	
Rt-Q-BOND		Restek	TG-BOND Q	
Rt-QS-BOND		Restek	TG-BOND Q+	
Rt-S-BOND		Restek	TG-BOND S	
Rt-U-BOND		Restek	TG-BOND U	
Supel-Q-PLOT		Supelco	TG-BOND Q	

# GC Column Selection by Application

- Recommended
- Alternative

	TG-1MS, TG-1MT, TR-1MS	TG-5MS, TG-5SIMS, TG-5MS AMINE, TG-5MT, TR-5, TR-5MS	TG-35MS, TG-35MS AMINE, TR-35MS	TG-17MS, TG-17SIMS	TG-130IMS	TG-170IMS, TR-170I	TG-WaxMS, TG-WaxMT, TR-Wax, TR-WaxMS	TG-WaxMS A	TG-WaxMS B	TG-Dioxin	TG-POLAR	TG-624, TG-624SIMS	TG-200MS	TG-225MS	TG-5HT, TR-5HT	TG-XLBMS	TG-VRX, TG-VMS	TG-OCP I, TG-OCP II	TG-OPP I, TG-OPP II	TG-ALC Plus I, TG-ALC Plus II	TR-FFAP	TR-VI	TR-FAME	TR-Simdist	TR-524	TR-525	TR-8270	TR-DoA5	TR-DoA35	TR-Biodiesel (M)	TR-Biodiesel (F)	TR-Biodiesel (G)	TR-Dioxin 5MS	TR-Pesticide, TR-Pesticide II, TR-Pesticide III, TR-Pesticide IV	TR-PCB 8MS	TR-8095			
Acids		●					●	●												●																			
Acid/Neutral Drugs		●	●																																				
Alcohols		●			●		●	●	●	●	●	●	●								●	●																	
Alcohols in Beverages					●		●	●	●	●	●	●									●	●																	
Aldehydes							●	●	●	●	●										●	●																	
Alditol Acetates (sugars)		●					●	●	●	●				●							●	●		●															
Amines – Aliphatic		●	●			●	●	●	●	●	●	●										●	●																
Amines – Aromatic		●	●			●	●	●	●	●	●	●										●	●																
Antidepressants		●	●			●	●	●	●	●	●	●										●	●																
Benzenes, substituted															●																								
Biodiesel – Methanol																																							
Biodiesel – FAMEs												●																											
Biodiesel – Glycerine																																							
Blood Alcohols											●										●	●																	
Brominated Flame Retardants			●																																				
Butter Fat			●												●																								
Carboxylic Acids									●																														
Cigarette Lighter Fuel			●																																				
Chlorinated Aromatics	●	●	●			●								●																									
Dioxins		●	●			●				●																													
Drugs of Abuse			●																																				
Drugs of Abuse – THC																																							
Essential Oils							●	●	●												●	●																	
Explosives																																							
FAMEs											●				●	●																							
Glucose – Methylated																																							
Herbicides		●	●			●																																	
Hydrocarbons																																							
Ketones						●	●	●	●	●	●	●	●	●								●	●																
Monomers						●																																	
Nitroaromatics			●			●	●	●	●	●	●	●																											
Organic Acids									●																														
Organochlorine Pesticides	●	●	●			●															●	●																	
Organophosphorous Pesticides	●	●	●			●																																	
PAHs	●	●	●			●																																	
Paraffins	●	●	●																																				
PCBs		●																																					
Pesticides																																							
Petroleum																																							
Phenols			●			●																																	
Phthalates	●	●																																					
Plant Sterols		●	●			●																																	
Polyethylene																																							
Polymers		●																																					
Polywax	●	●	●																																				
Pyrethroids	●	●	●																																				
Sedatives			●																																				
Semivolatiles	●	●																																					
Silicon Oil																																							
Solvents						●		●	●	●	●	●	●																										
Terpenes			●																																				
Triglycerides			●																																				
TRPH	●	●																																					
Volatiles		●	●			●		●	●	●	●	●	●																										
Xylenes	●	●					●	●	●																														

## GC Column Selection by U.S. Pharmacopeia Specifications

The USP specifications are listed below with the appropriate Thermo Scientific GC column offerings included for your convenience. In some cases, there is more than one phase that matches the phase description. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

USP Code	Description	Recommended Thermo Scientific Phase(s)
<b>G1</b>	Dimethylpolysiloxane oil	TG-1MS
		TG-1MT
		TR-1MS
<b>G2</b>	Dimethylpolysiloxane gum	TG-1MS
		TG-1MT
		TR-1MS
<b>G3</b>	50% Phenyl-50% Methylpolysiloxane	TG-17MS
		TR-50MS
		TG-17SiIMS
<b>G5</b>	3-Cyanopropylpolysiloxane	TR-FAME
<b>G6</b>	Trifluoropropyl Methylpolysiloxane	TG-200MS
<b>G7</b>	50% Cyanopropyl Phenylmethyl Polysiloxane	TG-225MS
<b>G16</b>	Polyethylene Glycol Compound (ave. mol. wt. ~15,000) with Diepoxide Linker	TG-WaxMS
		TG-WaxMT
		TR-WaxMS
		TR-Wax
<b>G19</b>	50% Cyanopropyl 50% Phenylmethyl Polysiloxane	TG-225MS
<b>G20</b>	Polyethylene Glycol (ave. mol. wt. of 380 – 420)	TG-WaxMS
		TG-WaxMT
		TR-WaxMS
		TR-Wax
<b>G27</b>	5% Phenyl-95% Methylpolysiloxane	TG-5MS
		TG-5MT
		TR-5MS
		TR-5
<b>G36</b>	1% Vinyl-5% Phenylmethylpolysiloxane	TR-5MS
		TR-5
<b>G38</b>	Phase G1 containing a small percentage of tailing inhibitor	TG-5MS
		TG-5MT
		TR-5MS
		TR-5
<b>G42</b>	35% Phenyl-65% Dimethylpolysiloxane (percentages refer to molar substitution)	TG-35MS
		TR-35MS
<b>G43</b>	6% Cyanopropylphenyl-94% Dimethylpolysiloxane (percentages refer to molar substitution)	TG-624
		TR-V1
		TG-624SiIMS
<b>G46</b>	14% Cyanopropylphenyl-86% Methylpolysiloxane	TG-1701MS
		TR-1701
<b>G48</b>	90% Biscyanopropyl 10% Cyanopropyl Phenyl Polysiloxane	TG-POLAR

## GC Column Selection by ASTM Method

Selected ASTM methods are listed below with the appropriate Thermo Scientific GC column offerings. In some cases, there is more than one phase or column dimension that can be used. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
<b>D1983</b>	Fatty acid methyl ester composition	TG-WaxMS	<b>26088-1420</b>
<b>D2245</b>	Oils and oil acids in solvent-reducible paints	TR-FAME	<b>260M154P</b>
<b>D2268</b>	High-purity n-heptane and isooctane	TG-1MS	<b>Inquire</b>
<b>D2306</b>	C8 aromatic hydrocarbons	TG-WaxMS	<b>26088-1540</b>
<b>D2360</b>	Trace impurities in monocyclic aromatic hydrocarbons	TG-WaxMS	<b>26088-1550</b>
<b>D2456</b>	Polyhydric alcohols in alkyd resin	TG-WaxMS	<b>26088-2980</b>
<b>D2580</b>	Phenols in water	TG-5MS	<b>26098-2230</b>
<b>D2753</b>	Oil and oil acids	TR-FAME	<b>260M154P</b>
<b>D2800</b>	FAME analysis	TR-FAME	<b>260M154P</b>
<b>D2804</b>	Purity of methyl ethyl ketone	TG-WaxMS	<b>26088-2980</b>
<b>D2887</b>	Boiling range distribution of petroleum fractions	TR-SimDist	<b>260S348P</b>
<b>D2998</b>	Polyhydric alcohols in alkyd resin	TG-1MS	<b>26099-2970</b>
<b>D2999</b>	Monopentaerythritol in commercial pentaerythritol	TG-1MS	<b>Inquire</b>
<b>D3009</b>	Composition of turpentine	TG-WaxMS	<b>26088-2240</b>
<b>D3054</b>	Cyclohexane	TG-1MS	<b>Inquire</b>
<b>D3168</b>	Polymers in emulsion paints	TG-1MS	<b>26099-2970</b>
<b>D3257</b>	Aromatics in mineral spirits	TG-624	<b>26085-3960</b>
<b>D3271</b>	Solvent analysis in paints	TG-WaxMS	<b>26088-2980</b>
<b>D3304</b>	PCBs in environmental materials	TG-5MS TR-PCB 8MS	<b>26098-1540</b> <b>26AJ148P</b>
<b>D3329</b>	Purity of methyl isobutyl ketone	TG-WaxMS TG-624	<b>26088-2980</b> <b>26085-3960</b>
<b>D3432</b>	Unreacted toluene diisocyanates in urethane prepolymers and coating solutions	TG-1MS	<b>26099-3090</b>
<b>D3447</b>	Purity of halogenated organic solvents	TG-624	<b>26085-3960</b>
<b>D3452</b>	Identification of rubber	TG-1MS	<b>26099-3090</b>
<b>D3457</b>	FAME analysis	TR-FAME	<b>260M154P</b>
<b>D3534</b>	PCBs in water	TG-5MS TR-PCB 8MS	<b>26098-3360</b> <b>26AJ148P</b>
<b>D3545</b>	Alcohol content and purity of acetate esters	TG-624	<b>26085-3960</b>
<b>D3687</b>	Alcohol content and purity of acetate esters	TG-WaxMS	<b>26088-2980</b>
<b>D3695</b>	Volatile alcohols in water by direct aqueous-injection GC	TG-WaxMS	<b>26088-2980</b>
<b>D3710</b>	Boiling range distribution of gasoline and gasoline fractions	TR-SimDist	<b>260S348P</b>
<b>D3725</b>	Fatty acids in drying oils	TR-FAME	<b>Inquire</b>
<b>D3760</b>	Isopropylbenzene (cumene)	TG-WaxMS TG-1MS	<b>26088-1550</b> <b>Inquire</b>
<b>D3797</b>	o-Xylene	TG-WaxMS	<b>26088-2360</b>
<b>D3798</b>	p-Xylene	TG-WaxMS	<b>26088-2360</b>
<b>D3871</b>	Purgeable organic compounds in water using headspace sampling	TG-624	<b>26085-4080</b>
<b>D3893</b>	Purity of methyl amyl ketone and methyl isoamyl ketone	TG-624	<b>26085-3960</b>
<b>D3973</b>	Low molecular weight halogenated hydrocarbons in water	TG-624	<b>26085-3960</b>
<b>D4059</b>	PCBs in insulating liquids	TG-5MS TR-PCB 8MS	<b>26098-1540</b> <b>26AJ148P</b>
<b>D4415</b>	Dimer in acrylic acid	TG-WaxMS	<b>26088-1430</b>

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
D4443	Residual vinyl chloride monomer content in ppb range in homo- and co-polymers by headspace GC	TG-624	26085-3960
D4735	Trace thiophene in refined benzene	TG-WaxMS	26088-2250
D4773	Propylene glycol monomethyl ether, dipropylene glycol monomethyl ether, and propylene glycol monomethyl ether acetate	TR-5	260E470P
D4806	Denatured fuel ethanol for blending with gasoline for use as automotive spark-ignition engine fuel	TG-1MS	Inquire
D4864	Traces of methanol in propylene concentrates	TG-5MS	Inquire
D4947	Chlordane and heptachlor in indoor air	TG-5MS	26098-3360
D5060	Impurities in high-purity ethylbenzene	TG-WaxMS	26088-2360
D5075	Nicotine in indoor air	TG-5MS	26098-2970
D5134	Petroleum naphthas through n-nonane	TG-1MS	Inquire
D5135	Styrene	TG-WaxMS	26088-2360
D5399	Boiling point distribution of hydrocarbon solvents	TR-SimDist	260S348P
D5441	Methyl t-butyl ether	TG-1MS	Inquire
D5442	Petroleum waxes	TG-1MS TG-5MS	26099-1430 26098-1300
D5480	Motor oil volatility	TG-5MS	Inquire
D5501	Ethanol content of denatured fuel ethanol	TG-1MS	Inquire
D5599	Oxygenates in gasoline by oxygen selective FID	TG-1MS	26099-3080
D5623	Sulfur compounds in light petroleum liquids using sulfur selective detection	TG-1MS	Inquire
D5713	High purity benzene for cyclohexane feedstock	TG-1MS	Inquire
D5739	Oil spill source identification using positive ion electron impact low resolution MS	TG-5MS	26098-1420
D5769	Benzene, toluene and total aromatics in finished gasolines	TG-1MS TG-624 TG-624SiIMS	26099-3080 26085-3330 26059-3330
D5790	Purgeable organic compounds in water	TG-5MS	26098-1420
D5812	Organochlorine pesticides in water	TG-1701MS TG-17MS TG-WaxMS	26090-1420 26089-1420 26088-1550
D5917	Trace impurities in monocyclic aromatic hydrocarbons	TR-FAME	260M154P
D5974	Fatty and rosin acids in tall oil fraction products	TG-1MS	Inquire
D5986	Oxygenates, benzene, toluene, C8-C12 aromatics and total aromatics in finished gasoline by GC/FTIR	TG-5MS	26098-1420
D6160	PCBs in waste materials	TR-SimDist	260S250P
D6352	Boiling range distribution of petroleum fractions	TG-1MS TR-SimDist	Inquire 260S250P
D6417	Engine oil volatility	TG-1MS	Inquire
D6584	Free and Total Glycerin in B-100 Biodiesel	TR-BioDiesel (G)	26AF024P
D6729	Individual components in spark ignition engine fuels	TG-1MS	Inquire
D6730	Individual components in spark ignition engine fuels using precolumn	TG-5MS TG-624	26098-2960 26085-4080
E202	Ethylene glycols and propylene glycols	TR-5	260E470P
E475	Di-tert-butyl peroxide	TG-1MS	Inquire
E1616	Acetic anhydride	TG-WaxMS	26088-3090
E1863	Acrylonitrile	TR-SimDist	260S250P

## GC Column Selection by U.S. EPA Drinking Water Test Method

Selected EPA Drinking Water methods are listed below with the appropriate Thermo Scientific GC column offerings. In some cases, there is more than one phase or column dimension that can be used. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
501.3	Trihalomethanes	TG-624	26085-3960
502.1	Volatile halogenated compounds	TG-624 TR-5MS	26085-4080 260F396P
502.2	Volatile organic compounds	TG-624 TG-624	26085-4080 26085-3320
503.1	Volatile aromatic and unsaturated organics	TG-624 TR-5MS	26085-4080 260F396P
504	EDB and DBCP	TR-5MS TG-5MS	260F396P 26098-2240
504.1	EDB and DBCP	TR-5MS TG-5MS	260F396P 26098-2240
506	Phthalates and adipates	TG-1MS TG-5MS	26099-1430 26098-1430
507	Organonitrogen and organophosphorus pesticides	TG-5MS TG-5MT TG-17MS TG-17SiIMS	26098-1420 26M98-1420 26089-1420 26072-1420
509	Ethylene thiourea	TG-1701MS TG-WaxMS	26090-1420 26088-1300
513	Dioxin	TG-5MS TG-5MT	26098-1540 26M98-1540
515.2	Chlorinated herbicides	TG-5MS TG-17MS	26098-1430 26089-1430
524.1	Volatile organic compounds	TR-524 TG-624 TG-624 TG-624SiIMS TG-624SiIMS	26RV495P 26085-4080 26085-3320 26059-4080 26059-3320
524.2	Volatile organic compounds	TR-524 TG-624 TG-624	26RV495P 26085-4080 26085-3320
525.1	Semi-volatile organic compounds	TR-525 TG-5MS TG-624SiIMS TG-624SiIMS	26RX142P 26098-1420 26059-4080 26059-3320
525.2	Semi-volatile organic compounds	TR-525 TG-5MS	26RX142P 26098-1420
527	Selected pesticides and flame retardants	TR-527 TG-5MS	26RF142P 26098-1420
548.1	Endothall	TG-1MS TG-5MS	26099-1430 26098-1420
551	Chlorinated disinfection by-products/chlorinated solvents	TG-5MS TG-1701MS	26098-1420 26090-2240
552	Haloacetic acids	TG-1701MS TG-35MS	26090-1430 26094-1430
552.1	Haloacetic acids and dalapon	TG-1701MS TG-35MS	26090-1430 26094-1430

## GC Column Selection by U.S. EPA Waste Water Test Method

Selected EPA Waste Water methods are listed below with the appropriate Thermo Scientific GC column offerings. In some cases, there is more than one phase or column dimension that can be used. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
601	Purgeable halocarbons	TG-624	26085-4080
		TG-624	26085-3320
602	Purgeable aromatics	TG-624	26085-4080
		TG-5MS	26098-2960
		TG-5MT	26M98-2960
603	Acrolein and acrylonitrile	TG-624	26085-4080
		TG-5MS	26098-2960
		TG-5MT	26M98-2960
604	Phenols	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
606	Phthalate ester	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
607	Nitrosamines	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
608.1	Organochlorine pesticides in industrial and municipal water	TG-5MS	26098-2240
608.2	Organochlorine pesticides in wastewater	TG-5MS	26098-2240
609	Nitroaromatics and isophorone	TG-5MS	26098-1430
		TG-35MS	26094-1430
610	Polynuclear aromatic hydrocarbons	TG-5MS	26098-1420
		TG-5MT	26M98-1420
611	Haloethers	TG-5MS	26098-1430
		TG-35MS	26094-1430
612	Chlorinated hydrocarbons	TG-5MS	26098-1430
		TG-35MS	26094-1430
613	Dioxin	TG-5MS	26098-1540
		TG-5MT	26M98-1540
614	Organophosphorous pesticides in industrial and municipal water	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-17MS	26089-1420
		TG-17SiIMS	26072-1420
614.1	Organophosphorous pesticides in wastewater	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-17MS	26089-1420
615	Chlorinated herbicides in industrial and municipal water	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-17MS	26089-1420
616	C, H, and O compounds	TG-1MS	26099-1420
		TG-5MS	26098-1420
		TG-5MT	26M98-1420
617	Organohalide pesticides and PCBs in industrial and municipal water	TG-5MS	26098-1420
		TG-5MT	26M98-1420
618	Volatile pesticides in industrial and municipal water	TG-1MS	26099-2240
		TG-5MS	26098-2240
619	Triazines, pesticides and PCBs in industrial and municipal water	TG-35MS	26094-1430
620	Diphenylamine in industrial and municipal water	TG-1MS	26099-1430
		TG-5MS	26098-1430
622	Organophosphorous pesticides in industrial and municipal water	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-17MS	26089-1420



GC Column Selection by U.S. EPA Waste Water Test Method *continued*

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
622.1	Thiophosphate pesticides	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
624	Purgeables	TG-624	26085-4080
		TG-624	26085-3320
		TG-624SiIMS	26059-4080
		TG-624SiIMS	26059-3320
625	Base/neutrals and acids	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-5MS	26098-1430
627	Dinitroaniline pesticides in industrial and municipal water	TG-5MS	26098-1430
		TG-35MS	26094-1430
630.1	Dithiocarbamate pesticides such as carbon disulfide	TG-5MS	26098-1420
		TG-5MS	26098-1430
		TG-5MT	26M98-1420
633	Organonitrogen pesticides	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-17MS	26089-1420
		TG-17SiIMS	26072-1420
633.1	Neutral nitrogen-containing pesticides	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
634	Thiocarbamate pesticides	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
645	Amine pesticides and lethane in industrial and municipal water	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420
646	Dinitro aromatic pesticides	TG-5MS	26098-1420
		TG-5MT	26M98-1420
		TG-35MS	26094-1420

## GC Column Selection by U.S. EPA Solid Waste Test Method

Selected EPA Solid Waste methods are listed below with the appropriate Thermo Scientific GC column offerings. In some cases, there is more than one phase or column dimension that can be used. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
8010B	Halogenated volatile organics	TG-624	26085-4080
		TG-624	26085-3320
8011	EDB and DBCP	TG-5MS	26098-1420
		TG-5MT	26M98-1420
8015B	Non-halogenated volatile organics	TG-624	26085-4080
		TG-5MS	26098-2960
		TG-5MT	26M98-2960
8020A	Aromatic volatile organics	TG-624	26085-4080
		TG-5MS	26098-2960
		TG-5MT	26M98-2960
8021A	Halogenated and aromatic volatile organics	TG-624	26085-4080
		TG-5MS	26098-2960
		TG-5MT	26M98-2960
8030A	Acrolein and acrylonitrile	TG-624	26085-4080
8031	Acrylonitrile	TG-624	26085-3390
8032	Acrylamide	TG-624	26085-3390

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
<b>8040A</b>	Phenols	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
		TG-35MS	<b>26094-1420</b>
<b>8060</b>	Phthalate esters	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
<b>8061</b>	Phthalate esters	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
<b>8070</b>	Nitrosamines	TG-5MS	<b>26098-1430</b>
<b>8081</b>	Organochlorine pesticides and PCBs	TG-5MS	<b>26098-2230</b>
		TG-5MT	<b>26M98-2230</b>
		TG-17MS	<b>26089-1420</b>
		TG-17SiIMS	<b>26072-1420</b>
<b>8090</b>	Nitroaromatics and cyclic ketones	TG-5MS	<b>26098-1430</b>
<b>8095</b>	Explosives	TR-8095	<b>260P123P</b>
<b>8100</b>	Polynuclear aromatic hydrocarbons	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
<b>8110</b>	Haloethers	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
<b>8120A</b>	Chlorinated hydrocarbons	TG-5MS	<b>26098-1430</b>
<b>8121</b>	Chlorinated hydrocarbons	TG-5MS	<b>26098-1430</b>
<b>8140</b>	Organophosphorous pesticides	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
		TG-17MS	<b>26089-1420</b>
<b>8141A</b>	Organophosphorous pesticides	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
		TG-17MS	<b>26089-1420</b>
<b>8150B</b>	Chlorinated herbicides	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
		TG-17MS	<b>26089-1420</b>
<b>8151</b>	Chlorinated herbicides	TG-5MS	<b>26098-1420</b>
		TG-5MT	<b>26M98-1420</b>
		TG-17MS	<b>26089-1420</b>
<b>8240B</b>	Volatile organic compounds	TG-624	<b>26085-4080</b>
		TG-624	<b>26085-3320</b>
		TG-624SiIMS	<b>26059-4080</b>
		TG-624SiIMS	<b>26059-3320</b>
<b>8250A</b>	Semi-volatile organic compounds	TG-5MS	<b>26098-1420</b>
		TG-5MS	<b>26098-1430</b>
		TG-5MT	<b>26M98-1420</b>
<b>8260A</b>	Volatile organic compounds	TG-624	<b>26085-4080</b>
		TG-624	<b>26085-3320</b>
<b>8270B</b>	Semi-volatile organic compounds	TG-5MS	<b>26098-1420</b>
		TG-5MS	<b>26098-1430</b>
		TG-5MT	<b>26M98-1420</b>
<b>8270C</b>	Semi-volatile organic compounds	TR-8270	<b>26RF296P</b>
<b>8280</b>	Polychlorinated dioxins and furans	TG-5MS	<b>26098-1540</b>
		TG-5MT	<b>26M98-1540</b>
<b>8290</b>	Polychlorinated dioxins and furans	TG-5MS	<b>26098-1540</b>
		TG-5MT	<b>26M98-1540</b>

## GC Column Selection by NIOSH Method

Selected NIOSH methods are listed below with the recommended Thermo Scientific GC column offerings included for your convenience. There may be more than one phase or column dimension that can be used. When in doubt, it is recommended that you consult the original complete method or contact our technical support team for additional information or help in choosing the correct column for your application.

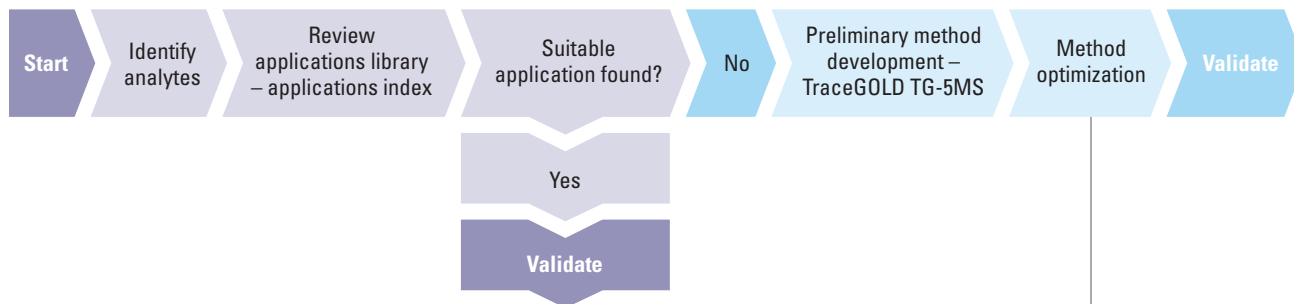
Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
801	Aerobic bacteria	TR-FAME	<b>Inquire</b>
1001	Methylene chloride	TG-1MS	<b>26099-1430</b>
1002	Chloroprene	TG-1MS	<b>26099-2960</b>
		TG-1MT	<b>26M99-2960</b>
1003	Halogenated hydrocarbons	TG-624	<b>26085-3390</b>
		TG-624SiMS	<b>26059-3390</b>
1004	Dichloroethyl ether	TG-1MS	<b>Inquire</b>
1005	Methylene chloride	TG-WaxMS	<b>26088-1430</b>
1010	Epichlorohydrin	TG-WaxMS	<b>Inquire</b>
1011	Ethyl bromide	TG-WaxMS	<b>26088-2240</b>
1013	Propylene dichloride	TG-WaxMS	<b>Inquire</b>
1015	Vinylidene chloride	TG-624	<b>Inquire</b>
1016	1,1,2,2-Tetrachloro-2,2-difluoroethane and 1,1,2,2-tetrachloro-1,2-difluoroethane	TG-WaxMS	<b>26088-2240</b>
1018	Dichlorodifluoromethane, 1,2-dichlorotetrafluoroethane and chlorodifluoromethane	TG-1MS	<b>26099-2970</b>
1020	1,1,2-Trichloro-1,2,2-trifluoroethane	TG-WaxMS	<b>26088-1430</b>
1300	Ketones 1	TG-WaxMS	<b>26088-2240</b>
1301	Ketones 2	TG-WaxMS	<b>26088-2240</b>
1302	N-Methyl-2-pyrrolidone	TG-5MS	<b>26098-2970</b>
1400	Alcohols 1	TG-WaxMS	<b>26088-2240</b>
1401	Alcohols 2	TG-WaxMS	<b>26088-2240</b>
1402	Alcohols 3	TG-WaxMS	<b>26088-2240</b>
1403	Alcohols 4	TG-WaxMS	<b>26088-1430</b>
1450	Esters 1	TG-WaxMS	<b>26088-2240</b>
1451	Methyl cellosolve acetate	TG-5MS	<b>26098-2970</b>
1453	Vinyl acetate	TG-5MS	<b>26098-2970</b>
1454	Isopropyl acetate	TG-1MS	<b>26099-2970</b>
1457	Ethyl acetate	TG-WaxMS	<b>26088-2970</b>
1458	Methyl acetate	TG-WaxMS	<b>26088-2970</b>
1501	Aromatic hydrocarbons	TG-WaxMS	<b>26088-2970</b>
1550	Naphthas	TG-1MS	<b>26099-1540</b>
		TG-1MT	<b>26M99-1540</b>
1551	Turpentine	TG-1MS	<b>26099-1540</b>
		TG-1MT	<b>26M99-1540</b>
1552	Terpenes	TG-WaxMS	<b>26088-3100</b>
1601	1,1-Dichloro-1-nitroethane	TG-1MS	<b>Inquire</b>
1602	Dioxane	TG-5MS	<b>26098-2970</b>
1604	Acrylonitrile	TG-WaxMS	<b>26088-2240</b>
1606	Acetonitrile	TG-WaxMS	<b>26088-2970</b>
1608	Glycidol	TG-WaxMS	<b>Inquire</b>
1609	Tetrahydrofuran	TG-WaxMS	<b>26088-2240</b>
1610	Ethyl ether	TG-1MS	<b>26099-2970</b>
1611	Methylal	TG-WaxMS	<b>Inquire</b>
1612	Propylene oxide	TG-5MS	<b>26098-2970</b>
1613	Pyridine	TG-5SiMS	<b>26096-2970</b>
1614	Ethylene oxide	TG-WaxMS	<b>Inquire</b>
1615	Methyl-tert-butyl ether	TG-1MS	<b>26099-2240</b>
2000	Methanol	TG-35MS	<b>26094-2980</b>
2004	Dimethylacetamide and dimethylformamide	TG-WaxMS	<b>26088-2240</b>

Method	Title	Recommended Thermo Scientific Phase(s)	Part Number
2005	Nitroaromatics	TG-5MS	26098-2250
		TG-5MT	26M98-2250
2007	Aminoethanol compounds 1	TG-5MS	Inquire
2010	Aliphatic amines	TG-5MS	26098-1420
		TG-5MT	26M98-1420
2012	n-Butylamine	TG-5MS	26098-1420
		TG-5MT	26M98-1420
2017	Aniline, o-toluidine and nitrobenzene	TG-5MS	26098-2970
2500	Methyl ethyl ketone	TG-1MS	26099-2970
2505	Furfuryl alcohol	TG-1MS	26099-1420
		TG-1MT	26M99-1420
2520	Methyl bromide	TG-1MS	26099-2970
2529	Furfural	TG-5MS	26098-2960
		TG-5MT	26M98-2960
2536	Valeraldehyde	TG-5MS	26098-1310
2537	Methyl methacrylate	TG-35MS	26094-2980
2541	Formaldehyde	TG-WaxMS	26088-2240
2542	Mercaptans	TG-1MS	26099-2960
		TG-1MT	26M99-2960
2546	Cresols and phenol	TG-WaxMS	26088-1430
2549	Volatile organic compounds (screening)	TG-1MS	26099-2960
		TG-1MT	26M99-2960
2550	Benzothiazole in asphalt fume	TG-1MS	26099-2970
2551	Nicotine	TG-5MS	26098-2970
3511	Monomethylaniline	TG-5MS	26098-1420
		TG-5MT	26M98-1420
3513	Tetranitromethane	TG-1MS	26099-1420
		TG-1MT	26M99-1420
5020	Dibutyl phthalate and di(2-ethylhexyl) phthalate	TG-1MS	26099-1300
		TG-1MT	26M99-1300
5515	Polynuclear aromatic hydrocarbons	TG-1MS	26099-3090
5519	Endrin	TG-1MS	26099-3090
5523	Glycols	TG-35MS	26094-2980
5600	Organophosphorus pesticides	TG-5MS	26098-2970
5602	Chlorinated organonitrogen herbicides (air sampling)	TG-17MS	26089-1420
		TG-17SiMS	26072-1420
5701	Resorcinol	TG-1MS	26099-1420
		TG-1MT	26M99-1420
9200	Chlorinated organonitrogen herbicides (hand wash)	TG-17MS	26089-1420
		TG-17SiMS	26072-1420
9201	Chlorinated organonitrogen herbicides (dermal patch)	TG-17MS	26089-1420
		TG-17SiMS	26072-1420

# GC Technical Information

## GC Method Selection and Optimization

The following flow chart briefly describes the common steps in GC method development and optimization.



Method optimization			
Improve sensitivity	Increase retention	Improve resolution	Increase speed
<b>Increase injection volume</b>	<b>Reduce temperature ramp rate</b> Increases the distribution co-efficient and increases analyte dwell time in the stationary phase	<b>Reduce temperature ramp rate</b> Increases the distribution co-efficient and increases analyte dwell time in the stationary phase	<b>Increase temperature ramp rate</b> Reduces the distribution constant, analytes spend less time in the stationary phase
<b>Reduce film thickness</b> Produces sharper peaks	<b>Reduce carrier linear flow rate</b> Increases interaction with the stationary phase. Increases retention and resolution, but also peak broadening.	<b>Reduce carrier linear flow rate</b> Increases interaction with the stationary phase. Increases retention and resolution, but also peak broadening.	<b>Increase carrier linear flow rate</b> Decreases interaction with the stationary phase
<b>Reduce column diameter</b> Reduces HETP and increases pressure to maintain linear flow rate	<b>Increase film thickness</b> More interaction with the sample	<b>Change column dimensions</b> Longer column, smaller ID	<b>Shorter column</b> Shorter analysis time
	<b>Change the phase</b> More polar columns retain polar compounds better and vice versa	<b>Increase film thickness</b> Can provide discrimination based on time spent in stationary phase	<b>Decrease film thickness</b> Analytes spend less time in the stationary phase
	<b>Increase column length</b> Maintain linear velocity	<b>Change the phase</b> More polar columns retain polar compounds and vice versa providing analyte discrimination	<b>Consider UltraFast GC</b> Can reduce analysis time by a factor of 20

## GC Troubleshooting

Before you start any troubleshooting, it is essential to observe safe laboratory practices. Know the chemical and physical properties of any solvents used and have the appropriate Material Safety Data Sheets (MSDSs) readily available. All electrically powered instruments should be shut down and unplugged before starting. Eye protection should also be worn.

The following table lists common GC problems encountered, the possible causes and solutions for your quick reference.

Symptom	Cause	Recommended Solutions
<b>Baseline Related Problems</b>		
Baseline Drifting	Accumulation of stationary phase.	Remove the end section of the column.
	Carrier gas cylinder pressure too low to allow control.	Replace the carrier gas cylinder. Increase the pressure.
	Drifting carrier gas or combustion gas flows.	Check the gas controllers.
	Accumulation of impurities in the column.	Check impurity levels in the gas source. Use correct gas purity. Replace or install appropriate Gas Filters.
Baseline Falling	Carrier gas leak in the system.	Perform a leak test. Check the tightness of the connections on the carrier gas line.
	Column is baking out.	Allow enough time for the column to stabilize.
Baseline Falling Away Slowly After a High Initial Value	Purge valve left closed during acquisition.	Alter the GC program. See your GC user manual for details.
	Inadequate purge flow rate.	Increase the purge flow rate.
	Purge valve left closed for too long.	Shorten the purge time.
	Solvent tail peak.	Increase the solvent delay. Shorten the purge time.
	Pre-filters are dirty. (when using a quadrupole MS detector)	Contact your service representative.
Baseline Rising	Accumulation of impurities in the column.	Check impurity levels in the gas source. Use correct gas purity. Replace or install appropriate Gas Filters.
	Contaminated detector.	Check the detector and clean it.
	There is bleeding from the GC column.	Condition column. Change the column.
	Air is leaking into the system.	Trace and repair the leak.
Baseline Rising Under Temperature Program Control	Column contaminated.	Recondition the column.
Baseline High Standing Current	Carrier gas flow rate too high.	Reduce the carrier gas flow.
	Column contaminated.	Recondition the column.
	Contaminated gases.	Replace gas cylinders. Replace the gas filters.
	Excessive column stationary phase bleeding.	Check the oven temperature, ensuring that it doesn't exceed the column upper limit. Recondition the column. Replace the column.
	Loose connections.	Ensure that all interconnections and screw connections are tight.
Baseline Irregular Shape: Dip After Solvent Peak	Detector contaminated.	Bake out the detector. Clean the detector.
Baseline Irregular Shape: S-shaped	Excessive column bleed during column temperature programming.	Reduce the upper column temperature. Bake out the column. Install a high temperature column.
	Oxygen contamination is decomposing the stationary phase.	Install oxygen filters in the carrier gas line. Check the pneumatic and inlet systems for leaks. Use correct gas purity with low oxygen content.
Baseline High Frequency Noise	Contaminated detector.	Isolate the detector from the electronics. If noise disappears, clean the collector.
	Combustion gas flow too low or too high.	Check the detector gas flows.
	Column contaminated.	Condition the column.
	Contaminated detector gas supply.	Check the gas purity and install appropriate filters.
	Detector temperature higher than column maximum temperature.	Reduce the detector temperature to the column temperature upper limit.
Baseline Spiking	Loose column fittings.	Tighten fittings accordingly.
	Column too close to flame. (when using an FID)	Lower the column to the correct position (2-3mm below the tip of the jet).
	Dirty jet or detector.	Isolate the detector from the electronics. If the spiking disappears, clean the jet and the collector.
	FID temperature too low. (when using an FID)	Increase the FID temperature to at least 150°C.

Symptom	Cause	Recommended Solutions
<b>Peak-Related Problems</b>		
Peaks Broadening	Column flow too high.	Reduce the flow to slightly above optimum.
	Column flow too low.	Increase the flow to slightly above optimum.
	Split flow too low in split injection.	Increase the flow to 40-50mL/min.
	Column performances degraded.	Test the column at the optimum flow rate.
	Dirty injector.	Clean or replace the liner.
	Stationary phase accumulated in the outlet.	Remove the last two coils from the column.
	Detector base body temperature too low.	Increase the temperature to 5°C below the column maximum.
	The sample is overloading the column.	Reduce the amount and/or concentration of the sample.
Double Peaks	Injection speed too low.	Inject more rapidly in a smooth motion.
	Wrong autosampler injection speed or mode.	Use a higher speed.
Peak Fronting	Column or detector overloaded.	Decrease the injected amount. Decrease the analyte concentrations. Increase the split ratio.
	Column temperature too low.	Increase the temperature.
	Stationary phase too thin.	Use a thicker-film column.
	Poor injection technique.	Repeat, with better injection technique.
Ghost Peaks	Contaminated carrier gas.	Replace the cylinder. Replace the filter.
	Contamination from laboratory glassware.	Ensure the glassware is clean and contamination-free.
	Decomposition of injected sample.	Decrease the injection port temperature. Use the on-column injection technique.
	Dirty injection solution.	Carry out adequate clean-up of sample prior to injection.
Broad Ghost Peaks	Contaminated inlet or pneumatics.	Remove the column and bake out the inlet. Use a high-quality septum. Replace the split vent filter. Install an in-line filter between the pneumatics and the inlet.
	Incomplete elution of previous sample.	Increase the final oven program temperature or total run time. Increase the column flow rate.
Irregular, Chair-shaped Peaks	Solvent flooding of column.	Increase the initial oven temperature. Reduce the injection volume (On-column). Install a retention gap (On-column).
No Peaks After Solvent Peak	Carrier gas flow too high.	Reduce the carrier gas flow rate.
	Combustion gas flow incorrect.	Check the combustion gas flow.
	Detector contaminated.	Bake out or clean the detector.
	FID flame extinguished by solvent peak.	Check the detector temperature and that flame is lit.
	Too much sample injected.	Inject less sample.
	Incorrect column position in S/SL injector (too high).	Check the column position.
No Peaks at All	Clogged syringe needle.	Replace or repair the syringe.
	Column broken or disconnected.	Check the column and connections.
	Defective electrometer or amplifier.	Check electrometer or amplifier and associated connections. Replace if required.
	Defective recording device.	Replace the recording device.
	FID flame is out.	Clean FID jet, check detector gas flows and re-light flame.
	Incorrect column position in S/SL injector (too high).	Check the column position.
Sample Peak Tailing	Column degradation causing activity.	Inject a test mixture and evaluate the column.
	Column/oven temperature too low.	Increase the column/oven temperature. Do not exceed the recommended maximum temperature for the stationary phase.
	Column contaminated at inlet.	Trim first 10-20cm from column and re-install in injector.
	Glass wool or inlet liner causing activity.	Replace with fresh silanized wool and a clean inlet liner.
	Inlet temperature too low.	Increase the inlet temperature.
	Poor or obstructed column connections.	Remake the column inlet connection.
	Wrong stationary phase.	Replace the column according to the column manufacturer's literature.
Solvent Peak Tailing	Incorrect column position in inlet.	Reinstall the column.
	Initial oven temperature too high (On Column).	Reduce the initial oven temperature.
	Septum purge flow too low and/or split/splitless vent flow too low.	Check and adjust the septum purge and vent flows.
	Too large injection size.	Reduce the injection size.

GC Troubleshooting *continued*

Symptom	Cause	Recommended Solutions
Unresolved Peaks	Carrier gas flow rate too high.	Reduce the carrier gas flow rate.
	Column deteriorated.	Replace the column.
	Column temperature too high.	Lower the column oven temperature.
	Column too short.	Use a longer column.
	Incorrect column choice.	Install a suitable column.
	Injection technique is not adequate.	Choose a correct injection technique.
Discrete High-intensity Contaminant Peaks	Bleed from the GC column.	Condition or change the column.
	Bleed from the septum.	Replace the septum.
	Sample vial septa are contaminating the sample.	Discard sample. Store samples upright, in a refrigerator. Use Teflon™ faced septa, with the Teflon facing downwards (i.e. towards the sample).

**Results-Related Problems**

Low Reproducibility of Peak Area	Concentration not compatible with the dynamic range of the detection system.	Ensure that the sample concentration is suitable for the detection system.
	Inappropriate injection technique.	Try a different injection technique.
	Injection parameters inappropriate.	Check the injection temperature. Check the flow rates.
	Non reproducible sample injection technique.	Evaluate the sample preparation sequences. Compare the results with a series of standard injections.
	Leaking syringe or septum.	Check and replace the syringe at regular intervals. Check and replace septum at regular intervals.
	Leaks at the injection.	Check the column connections. Run a leak check.
	Poor injection technique.	Carefully meter the injected amount. Use a clean, good-quality syringe.
Poor split flow or ratio control.	Monitor the flow. Replace the in-line filter.	
Poor Sensitivity Increased Retention Time	Carrier gas flow rate too low.	Increase the carrier gas flow rate. Locate and remove possible obstructions in the carrier gas line. Check the injector/column ferrules.
Poor Sensitivity with Normal Retention Time	Oven or injector parameters are not optimized.	Adjust the oven parameters. Adjust the injector parameters.
	Leaks in the GC carrier gas line.	Run a leak test and correct leaks.
	Syringe leaks during injection.	Replace syringe or piston seals, if applicable.
	Split injection temperature too low.	Increase the temperature of the injector.
	Column is in poor condition, or wrong column type used.	Condition the columns. Change the column.
Retention Times Decreasing	Stationary phase deteriorated by oxygen and/or water.	Use a carrier gas free of oxygen and water. Replace or install appropriate gas filters.
	Stationary phase loss due to column bleeding.	Reduce the column temperature.
Retention Times Increasing	Increasing carrier leakage.	Check the septum and column connections.
	Carrier gas supply running out.	Replace the bottle.
Low Reproducibility of Retention Times	Drifting or unstable pneumatic controller.	Monitor the column pressure or flow. Check and replace the controller if necessary.
	Poor injection technique.	Start the run at consistent time after injection.
	Sample size is too large.	Reduce the injected amount and/or volume.
	Unstable column temperature.	Check the main oven door and cooling flap. Monitor the column temperature.
Retention Times are Inconsistent	GC column is in poor condition.	Condition the column. Change the column.
	Insufficient equilibration time set on GC.	Increase equilibration time.
	Poor injection.	Repeat with better injection technique.
	Oven temperature programmed to rise too quickly.	Reduce oven temperature ramp rate.
	Air is leaking into the system at the injector seal or the carrier gas manifold.	Trace and repair the leak.



## GC Equations

### Adjusted Retention Time ( $t_R'$ )

An analyte's retention time ( $t_R$ ) minus the elution time of an unretained peak ( $t_m$ ).

$$t_R' = t_R - t_m$$

Adjusted retention time is also equivalent to the time the analyte spends in the stationary phase.

### Capacity Factor ( $k$ )

Expression that measures the degree of retention of an analyte relative to an unretained peak, where  $t_R$  is the retention time for the sample peak and  $t_m$  is the retention time for an unretained peak. A measurement of capacity will help determine whether retention shifts are due to the column (capacity factor is changing with retention time changes) or the system (capacity factor remains constant with retention time changes).

$$k = \frac{t_R - t_m}{t_m}$$

Thus, the higher the capacity factor, the longer the retention time.

### Effective Theoretical Plates ( $N_{eff}$ )

A measure of a column performance that accounts for the effects of unretained elution time, where  $t_R'$  is the adjusted retention time and  $\sigma$  is the standard deviation of the peak.

$$N_{eff} = \left( \frac{t_R'}{\sigma} \right)^2$$

This value also remains constant as retention gaps and guards are used. Depending on the method of peak width calculation, different efficiencies can be reported. This leads to two popular measures:

$$N_{eff} = 16 \left( \frac{t_R'}{W} \right)^2$$

Where  $W$  is the tangential peak width (13.4% peak height).

$$N_{eff} = 5.54 \left( \frac{t_R'}{W} \right)^2$$

Where  $W$  is the width measured at half height (50% peak height).

### HEEP ( $H_{eff}$ )

Height Equivalent to an Effective Plate.

$$H_{eff} = L/N_{eff}$$

Where  $L$  is the column length. The smaller the  $N_{eff}$ , the more efficient the column's performance.

### HETP ( $H$ )

Height Equivalent to a Theoretical Plate is a measure of column efficiency where  $L$  is the column length and  $N$  is the number of theoretical plates.

$$H = L/N$$

HETP is based on actual ( $t_R$ ) rather than adjusted retention times ( $t_R'$ ).

### Linear Velocity ( $u$ )

Mobile phase flow rate expressed in cm/s and is expressed as:

$$u = L/t_m$$

Where  $L$  is the column length and  $t_m$  is the breakthrough time of an unretained peak.

### Phase Ratio ( $\beta$ )

The ratio of the volume of mobile phase to the stationary phase. An important value when changing the column dimensions in a method.

$$\beta = \frac{\text{column ID } (\mu\text{m})}{4 \times \text{film thickness } (\mu\text{m})}$$

### Resolution

A measure of the separation of two peaks taking into account both the difference in elution time and the peak widths.

$$R_s = \frac{(t_2 - t_1)}{0.5(W_1 + W_2)}$$

Where  $t_2$  and  $t_1$  are the two retention times, and  $W_1$  and  $W_2$  are baseline peak widths.

### Selectivity ( $\alpha$ )

The relative retention of two adjacent peaks. Selectivity can be calculated using capacity factor.

$$\alpha = \frac{k_2}{k_1}$$

### Trennzahl Number

A value to describe a separation. The Trennzahl number is calculated from the resolution between two consecutive homologous hydrocarbons. The Trennzahl number represents the number of peaks that can be included between the two hydrocarbon peaks.

$$T_z = \left( \frac{t_{R2} - t_{R1}}{(W_h)_1 + (W_h)_2} \right) - 1$$

Where  $t_R$  equals analyte retention time and  $W_h$  equals peak width at half height.

### van Deemter Equation

This is a relationship that considers the effect of linear velocity on the HETP or  $H$ , where  $A$  accounts for eddy diffusion,  $B$  describes the molecular diffusion of the vapor in the direction of the column axis,  $C$  refers to the resistance to transfer from the stationary to mobile phase and  $u$  is the linear velocity of the mobile phase.

$$H = A + \frac{B}{u} + C u$$

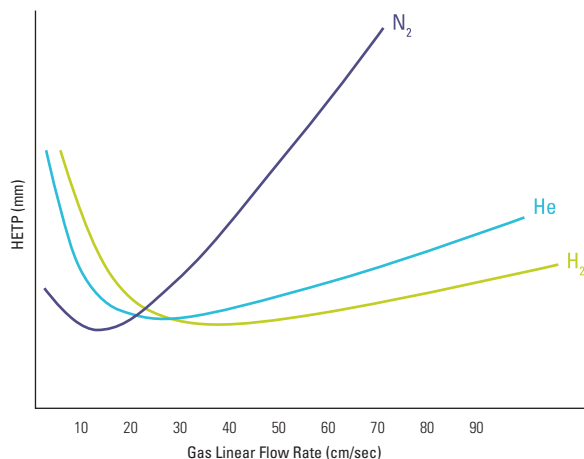
## Carrier Gas Choice

The choice of carrier gas is a compromise between a number of considerations, among them, efficiency and speed as well as availability, safety and cost. The three most common carrier gases used are nitrogen, helium and hydrogen.

Nitrogen shows the lowest HETP, making it the most efficient of the gases. High quality nitrogen is readily available and inexpensive compared to other options. However, the optimum flow rate to achieve nitrogen's very low HETP leads to long analysis times (see figure).

Helium has a slightly lower efficiency than nitrogen, but the optimum flow rate is higher. Also small changes in flow rate of helium around the optimum will not affect efficiency as greatly as with nitrogen.

For many, hydrogen is the carrier gas of choice. It shows higher efficiency than helium and at a higher flow rate. The variation in HETP with changes in flow rate is also far lower, making it more forgiving and reproducible. There is, however, a slight risk of an explosive atmospheric build-up in the oven.



A van Deemter plot of efficiency against linear flow rate for three carrier gases.

### Recommended Flow Rates and Velocities for Capillary Columns

Carrier Gas	0.25mm ID		0.32mm ID		0.53mm ID	
	mL/min	cm/min	mL/min	cm/min	mL/min	cm/min
He	1	35	1.7	35	6	35
H <sub>2</sub>	1.6	50	2.6	50	7.5	50
N <sub>2</sub>	0.4	14	0.5	11	0.9	7

### Recommended Detector Gas Flow Rates

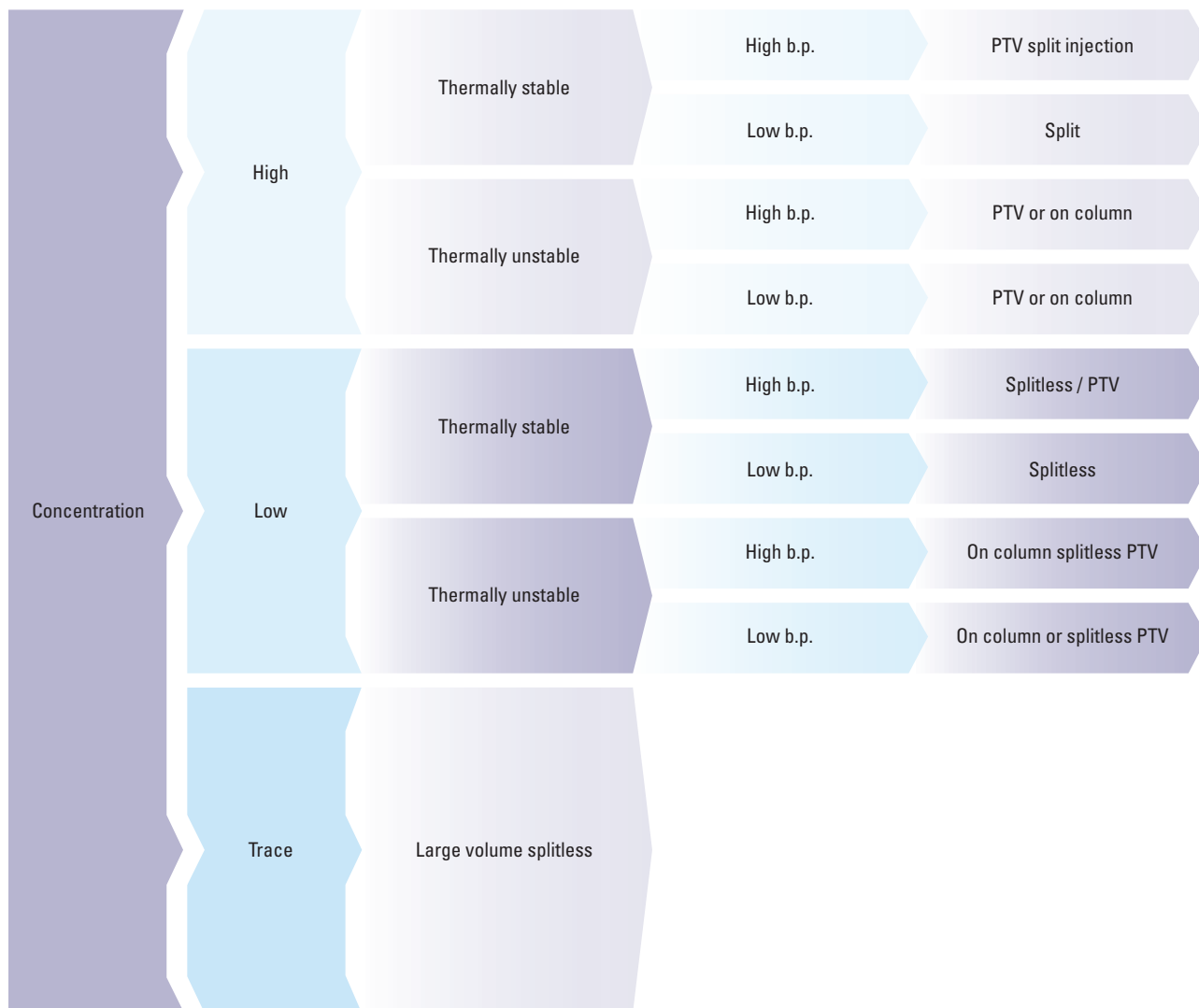
Detector	Air (mL/min)	H <sub>2</sub> (mL/min)	Make Up (mL/min)
ECD	–	–	35-40
FID	350	35	30
NPD	60	2.5	15
FPD	100	75	30

### Unretained Compounds

Detector	Analyte
FID	Methane
ECD	Methylene Chloride
NPD	Acetonitrile
TCD, MS	Methane, Butane
PID, ELCD	Vinyl Chloride

## Selection of Injection Method

The identification of the most appropriate injection method relies on the sample type and the boiling point to be used in the separation. The diagram below summarizes this selection process:



## Column Conditioning (All Columns Except TraceGOLD, TG-WaxMS, TRACE TR-1MS and TR-WaxMS)

It is recommended that before the column is subjected to any thermal gradients, all oxygen has been removed because the presence of oxygen in the system can shorten the column lifetime. Removal of oxygen can be achieved by purging the columns with oxygen-free carrier gas for a minimum of 20 minutes at 40°C using an approximate head pressure of 100kPa.

Although all Thermo Scientific columns have been pre-conditioned, we recommend that they are conditioned after installation by following these steps:

1. Heat the column from 50°C to the maximum operating temperature at 5°C/min. and hold for one hour. The maximum operating temperatures for all TRACE GC columns are provided below. It is important to stay within the maximum temperature range for the column.
2. Monitor the detector signal during conditioning until a stable baseline is reached. Due to the factory pre-conditioning of the column, this should be achieved in approximately one hour. This duration may be longer in the case of thick films and polar phases.

### Maximum Operating Temperatures for TraceGOLD and TRACE GC Columns

Column	Maximum Operating Temperature
TG-1MS	330°C / 350°C
TG-XLBMS	360°C
TG-5MS	330°C / 350°C
TG-SQC	330°C / 350°C
TG-5MS AMINE	300°C / 315°C
TG-5SILMS	330°C / 350°C
TG-5HT	380°C / 400°C
TG-35MS	300°C / 320°C
TG-35MS AMINE	220°C
TG-17MS	300°C / 320°C
TG-17SiIMS	340°C / 360°C
TG-1301MS	260°C / 280°C
TG-624	240°C
TG-624SiIMS	320°C
TG-VRX	260°C
TG-VMS	260°C
TG-1701MS	260°C / 280°C
TG-225MS	240°C
TG-200MS	320°C / 340°C
TG-POLAR	275°C
TG-WaxMS	260°C
TG-WaxMS A	250°C
TG-WaxMS B	220°C
TG-Dioxin	340°C
TG-OCP I / TG-OCP II	340°C
TG-OPP I / TG-OPP II	330°C
TG-ALC I / TG-ALC II	260°C
TG-1MT	430°C
TG-5MT	430°C
TG-WaxMT	260°C

Column	Maximum Operating Temperature
TR-1MS	340°C / 360°C
TR-5	320°C / 340°C for films ≤ 1.5µm 280°C / 300°C for films > 1.5µm
TR-5MS	360°C / 370°C for films ≤ 1.5µm 350°C / 360°C for films > 1.5µm
TR-5HT	380°C / 400°C
TR-35MS	330°C / 360°C
TR-1701	280°C / 300°C
TR-50MS	360°C / 370°C
TR-225	230°C / 250°C
TR-Wax	260°C / 280°C for films ≤ 1.0µm 240°C / 260°C for films > 1.0µm
TR-WaxMS	260°C / 280°C
TR-FFAP	240°C / 250°C
TR-SimDist	400°C for films ≤ 1.0µm 370°C for 2.65µm films
TR-V1	280°C / 300°C
TR-FAME	250°C / 260°C
TR-524	240°C / 260°C
TR-525	340°C / 360°C
TR-527	330°C / 350°C
TR-8095	360°C / 370°C
TR-8270	330°C / 350°C
TR-PCB 8MS	330°C / 350°C
TR-Dioxin 5MS	330°C / 350°C
TR-Biodiesel (M)	300°C / 320°C
TR-Biodiesel (F)	280°C / 300°C
TR-Biodiesel (G)	380°C / 400°C
TR-DoA5	330°C / 350°C
TR-DoA35	330°C / 350°C
TR-Pesticide	330°C / 350°C
TR-Pesticide II	330°C / 350°C
TR-Pesticide III	300°C / 320°C
TR-Pesticide IV	300°C / 320°C

## Column Conditioning for the TraceGOLD, TG-WaxMS, TRACE TR-WaxMS and TR-1MS Columns

This procedure will ensure an ultra low bleed for the column's entire lifetime and is only required once. Once performed, future installation of the column need only be followed by a 30-minute hold at the maximum temperature limit.

After installing the column according to the instrument manufacturer's instructions, follow the procedure below.

Steps	TG-WaxMS/TR-WaxMS	TR-1MS
1	Equilibrate the column at 40°C with carrier gas flow for 20 minutes, purging air content.	Equilibrate the column at 40°C with carrier gas flow for 20 minutes, purging air content.
2	Raise the temperature to 100°C at 5°C/min.	Raise the temperature to 100°C at 5°C/min.
3	Hold for 30 minutes.	Hold for 30 minutes.
4	Raise to 150°C at 5°C/min.	Raise to 150°C at 5°C/min.
5	Hold for 30 minutes.	Hold for 30 minutes.
6	Raise to 200°C at 5°C.	Raise to 250°C at 5°C.
7	Hold for 40 minutes.	Hold for 40 minutes.
8	Raise to 250°C at 5°C/min.	Raise to 300°C at 5°C/min.
9	Hold for 40 minutes.	Hold for 40 minutes.
10	Raise to 280°C at 5°C/min.	Raise to 360°C at 5°C/min.
11	Hold for 30 minutes.	Hold for 30 minutes.

Although quite a long procedure, it will result in longer lifetimes and lower bleed for your column.

## Performance Recovery

The performance of the column may exhibit signs of deterioration over time as a result of many different causes. Some of these, such as contamination by high boiling or strongly retained compounds, can be cleared by repeating the column-conditioning until a stable baseline is achieved.

Other contamination such as non-volatile compounds, pieces of septa or ferrule metal can result in poor peak shape due to band broadening at the injection step. This can be cured by the removal of a section from the front end of the column. The amount removed is dependent on the degree of contamination, the size of injection and the ID of the column,

but generally 50cm should be sufficient. As the efficiency of the column is proportional to the square root of its length, the removal of the front end will not lower the separation effectiveness by the same ratio as 50cm/column length. A last resort in column regeneration is column washing. Column washing uses a pressurized vessel to force solvent through the column in a reverse direction. The selection of the solvent is dependent on the nature of the samples that have been analyzed and therefore the contamination. It is also dependent on the stationary phase. Generally, 2mL of pentane is suitable for non-polar contamination with methanol used for more polar samples.

# GC Reagents

## Derivatization

Chemical literature contains an abundance of data on derivatization, most of which is relevant to particular compounds, classes of compounds and derivatization reagents. Two books are recognized as standards in the field of analytical derivatization. The first book, *Handbook of Analytical Derivatization Reactions* by Daniel R. Knapp<sup>1</sup>, provides a general collection of analytical derivatization methods for chromatography and mass spectrometry (MS) that involves formation of covalent derivatives prior to analysis. The second book, *Silylation of Organic Compounds* by Alan F. Pierce,<sup>2</sup> "was a significant factor in the transfer of silylation reactions from the relatively esoteric field of organosilicon chemistry to the status of perhaps the most widely practiced of derivatization methods."<sup>3</sup>

### Compounds or compound mixtures are derivatized before analysis for the following reasons:

1. To make a compound that otherwise could not be analyzed by a particular method suitable for analysis.<sup>4</sup>
2. To improve the analytical efficiency of the compound.<sup>5,6</sup>
3. To improve the detectability of the compound.<sup>7</sup>

## Suitability

Often compounds cannot be analyzed because they are not in a form that is suitable for the particular analytical technique. Examples include nonvolatile compounds for GC analysis,<sup>8,9,10</sup> insoluble compounds for HPLC analysis and materials that are not stable using the conditions of the technique.<sup>11</sup> The derivatization procedure modifies the chemical structure of the compounds, allowing analysis by a desired technique.<sup>12</sup>

## Efficiency

Direct analysis can be difficult when compounds interact with each other or with the column. These interactions can lead to poor peak resolution and/or asymmetrical peaks that make proper peak integration difficult or impractical. This interference can be reduced with conversion to derivatized products.<sup>13,14</sup> Compounds that exhibit co-elution can often be separated by using the appropriate derivatization methods.

## Detectability

As demand increases for the analysis of increasingly smaller amounts of materials, it becomes important to extend the detectability range of the materials in question. This increased sensitivity can be accomplished by improved detector design that is directed toward specific atoms or functional groups.

Another popular approach to increase detectability is the use of derivatization. Enhanced detectability can be achieved by increasing the bulk of the compound, or by introducing atoms or functional groups that strongly interact with the detector.<sup>16,17</sup> This technique is performed in gas chromatographic applications, with the addition of halogen atoms for electron capture detectors,<sup>18,19</sup> and with the formation of TMS derivatives to produce readily identifiable fragmentation patterns and mass ions.<sup>20</sup>

## Types of Derivatization

Compounds containing functional groups with active hydrogens (-COOH, -OH, -NH and -SH) are usually derivatized prior to analysis by gas chromatography. These functional groups have a tendency to form intermolecular hydrogen bonds that affect the volatility, their tendency to interact deleteriously with column packing materials and their thermal stability. Silylation, acylation and alkylation are derivatization techniques used to alter these functional groups to improve their thermal and chromatographic character.

### The ideal derivatization procedure will:

1. Accomplish the desired modification.
2. Proceed quantitatively, or at least reproducibly.
3. Produce products that are readily distinguishable and separable from the starting materials.
4. Proceed rapidly with simple and straightforward laboratory techniques that will be both selective and applicable to a number of similar compounds.
5. Involve reagents and reactions that present no unusual hazards.



## Thermo Scientific Silylation Reagents

Silyl derivatives are the most widely used derivatives for gas chromatographic applications. Usually they are formed by the replacement of the active hydrogens from acids, alcohols, thiols, amines, amides and enolizable ketones and aldehydes with the trimethylsilyl group. A variety of reagents is available for the introduction of the trimethylsilyl group. These reagents differ in their reactivity, selectivity and side reactions and the character of the reaction products from the silylation reagent itself. Considerable literature is available to assist you in the selection of the most suitable silylation reagent for your particular compounds or systems.<sup>1,2</sup>

Silylation reagents and trimethylsilyl derivatives are hydrolytically unstable and must be protected from moisture. However, the rate of hydrolysis for various reagents and derivatives is different, and sometimes it is possible to prepare derivatives in the presence of small amounts of moisture,<sup>21</sup> or to isolate and purify derivatives by extraction in an organic solvent, followed by washing with aqueous solutions.<sup>22</sup> Reagents that introduce a t-butyl dimethylsilyl group instead of the trimethylsilyl group were developed for greater hydrolytic stability.<sup>23</sup> These derivatives provide improved stability against hydrolysis and provide distinctive fragmentation patterns, making them useful in GC-MS applications.<sup>24</sup>

Most trimethylsilyl and t-butyl dimethylsilyl derivatives offer excellent thermal stability and are suitable for a wide range of injector and column conditions. However, as the silylation reagents will derivatize nearly all active hydrogens, it is important that they are not injected onto any column in which the stationary phase contains these functional groups. Examples of packings that are not compatible with silylating reagents are polyethylene glycols (TG-WaxMS) and free fatty acid phases (TG-WaxMS A).

### References

- Knapp D.R. (1979). *Handbook of Analytical Derivatization Reactions*, John Wiley & Sons: New York.
- Pierce, A.E. (1968). *Silylation of Organic Compounds*, Pierce Chemical: Rockford, IL.
- Pierce, A.E. (1968). *Silylation of Organic Compounds*, Pierce Chemical: Rockford, IL. p. 2.
- Sweeley, C.C., *et al.* (1963). Gas-liquid chromatography of trimethylsilyl derivatives of sugars and related substances. *J. Am. Chem. Soc.* **85**, 2495-2507.
- Khalifa, S. and Mumma, R.O. (1972). *J. Agric. Food Chem.* **20**, 632.
- Sinsheimer, J.E. and Smith, R.V. (1967). Methods for the qualitative and quantitative analysis of some hydroxystilbenes. *J. Pharm. Sci.* **56**, 1280.
- Poole, C.F. (1976). *Chem. Ind. (London)*, 479.
- Brittain, G.D. and Schewe, L. (1971). In *Recent Advances in Gas Chromatography*, Domsky, I.I. and Perry, J.A., Eds., Marcel Dekker: New York, NY.
- Sakauchi, N. and Horning, E.C. (1971). *Anal. Lett.* **4**, 41-42.
- Sullivan, J.E. and Schewe, L.R. (1977). Preparation and gas chromatography of highly volatile trifluoroacetylated carbohydrates using *N*-Methylbis (trifluoroacetamide). *J. Chromatogr. Sci.* **15**, 196-197.
- Hallgren, B. and Larsson, S. (1962). *J. Lipid Res.* **3**, 31.
- Samuelsson, K. and Samuelsson, B. (1969). Gas-liquid chromatography-mass spectroscopy of cerebrosides as trimethylsilyl ether derivatives. *Biochem. Biophys. Res. Commun.* **37**(1), 15-21.
- Langer, M., *et al.* (1960). *Chem. Ind. (London)*, **378**.
- Neeman, M., *et al.* (1959). *Tetrahedron*, **6**, 36.
- Marfey, P. (1984). Determination of D-amino acids. II. Use of a bifunctional reagent, 1,5-Difluoro-2,4-Dinitrobenzene. *Carlsberg Res. Commun.* **49**, 591-596.
- Ehrsson, H., *et al.* (1971). *Acta. Pharm. Suecica.* **8**, 319.
- Koshy, K.T., *et al.* (1975). *O*-(2,3,4,5,6-Pentafluorobenzyl) hydroxylamine hydrochloride as a sensitive derivatizing agent for the electron capture gas liquid chromatographic analysis of keto steroids. *J. Chromatogr. Sci.* **13**(Feb), 97-103.
- Walle, T. and Ehrsson, H. (1970). *Acta. Pharm. Suecica.* **7**, 389-406.
- Benington, F., *et al.* (1975). Identification and separation of indolealkylamines by gas liquid chromatographic analysis of their heptafluorobutryl derivatives. *J. Chromatogr.* **106**, 435-439.
- Kelly, R.W. and Taylor, P.L. (1976). *tert*-Butyldimethylsilyl ethers as derivatives for qualitative analysis of steroids and prostaglandins by gas phase methods. *Anal. Chem.* **48**(3), 465.
- Lau, H.L. (1966). *J. Gas Chromatogr.* **4**, 136.
- Tallent, W.H. and Kleinman, R. (1968). *J. Lipid Res.* **9**, 146.
- Mawhinney, T.P. and Madson, M.A. (1982). *N*-Methyl-*N*-(*tert*-butyldimethylsilyl) trifluoroacetamide and related *N*-*tert*-butyldimethylsilyl amides as protective silyl donors. *J. Org. Chem.* **47**, 3336-3339.
- Bazan, A.C. and Knapp, D.R. (1982). Improved derivative of 6-keto-prostaglandin F<sub>1α</sub> for gas chromatographic-mass spectrometric analysis. *J. Chromatogr.* **236**, 201-207.

## Thermo Scientific Acylation Reagents

Acylation is the conversion of compounds (through the action of a carboxylic acid or a carboxylic acid derivative) that contain active hydrogens such as -OH, -SH and -NH to esters; thioesters; and amides.<sup>1</sup> In chromatographic applications, the acylation reaction is used primarily for converting the above classes of compounds into derivatives that are better suited for chromatography<sup>2</sup> or that give a greater response to the chromatographic detection system than the parent compound.<sup>3</sup>

An important example of this application is the insertion of perfluoroacyl groups into a molecule to enhance the detectability of the substance by electron capture. The presence of a carbonyl group adjacent to the halogenated carbons enhances the electron capture detector (ECD) response.

Acyl derivatives are also useful in MS applications in which they influence the fragmentation patterns of the compounds to be studied.<sup>4</sup>

### References

1. Donike, M. (1973). Acylation with bis (acylamides). *N*-Methyl-bis (trifluoroacetamide), two new reagents for trifluoroacetylation. *J. Chromatogr.* **78**, 273-279.
2. Sullivan, J.E. and Schewe, L.R. (1977). Preparation and gas chromatography of highly volatile trifluoroacetylated carbohydrates using *N*-Methyl-bis (trifluoroacetamide). *J. Chromatogr. Sci.* **15**, 196-197.
3. Benington, F., *et al.* (1975). Identification and separation of indolealkylamines by gas liquid chromatographic analysis of their heptafluorobutyryl derivatives. *J. Chromatogr.* **106**, 435-439.
4. Borga, O., *et al.* (1971). Quantitative determination of nortriptyline and desmethylnortriptyline in human plasma by combined gas chromatography-mass spectrometry. *J. Chromatogr.* **4(12)**, 837-849.

## Thermo Scientific Alkylation Reagents

When used in derivatization for gas chromatography, alkylation represents the substitution of an active hydrogen by an aliphatic or aliphatic-aromatic<sup>1</sup> (benzyl) group. This technique is used to modify those compounds containing acidic hydrogens, such as carboxylic acids and phenols. The principal chromatographic use of this reaction is the conversion of organic acids into esters, which produce better chromatograms than the free acids.

In addition, alkylation reactions can be used to prepare ethers, thioethers and thioesters; *N*-alkylamines; and amides.<sup>2</sup> As the acidity of the active hydrogen decreases, the strength of the alkylating reagent must be increased. As the reagents and conditions become harsher, the selectivity and applicability of the methods become more limited.

### References

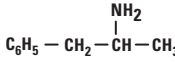
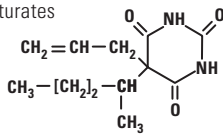
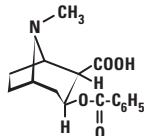
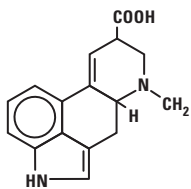
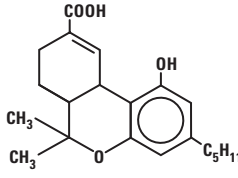
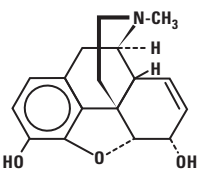
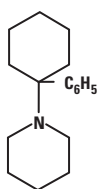
1. Kawahara, F.K. (1968). Microdetermination of derivatives of phenols and mercaptans by means of electron capture gas chromatography. *Anal. Chem.* **40(6)**, 1009.
2. Kananen, G., *et al.* (1972). Barbiturate analysis – a current assessment. *J. Chrom. Sci.* **10**, 283-287.



## Derivatization Reagents for Specific Functional Groups

Functional Group	Procedure	Reagent	Derivative	Notes	
<b>Amides</b> $\begin{array}{c} \text{O} \\    \\ \text{-C-NH}_2 \end{array}$ Primary	Silylation	BSA	TMS Amides	Difficult to form due to steric hindrance	
		BSTFA	TMS Amides		
		BSTFA+TMCS	TMS Amides		TMCS used as a catalyst
		MSTFA	TMS Amides		Reaction byproducts more volatile
		MSTFA+TMCS	TMS Amides		
	Secondary	Tri-Sil Reagents	TMS Amides		
		MTBSTFA	TBDMCS Amides	Difficult to form; very stable	
		MTBSTFA+TBDMCS	TBDMCS Amides	TBDMCS aids derivatization	
		MBTFA	Trifluoroacetamides		
		TFAA	Trifluoroacetamides		
Secondary	PFAA	Pentafluoropropionamides	Good for ECD detection		
	HFBI	Heptafluorobutyamides			
	Alkylation	MethElute Reagent (TMPAH)	Methyl Amides	On-column derivatization especially for drugs	
<b>Amines</b> $\begin{array}{c} \text{H} \\   \\ \text{-C-NH}_2 \\   \\ \text{H} \end{array}$ Primary	Silylation	BSA	TMS	TMCS aids derivatization	
		BSTFA	TMS		
		BSTFA+TMCS	TMS		
		MSTFA	TMS		
		MSTFA+TMCS	TMS		
	Secondary	Tri-Sil® Reagents	TMS		
		MTBSTFA	TBDMCS	Difficult to form, but more stable	
		MTBSTFA+TBDMCS	TBDMCS	TBDMCS aids derivatization	
		MBTFA	Trifluoroacetamides	Good for trace analysis with ECD	
		TFAA	Trifluoroacetamides	Good for trace analysis with ECD	
Secondary	TFAI	Trifluoroacetamides	Good for trace analysis with ECD		
	PFAA	Pentafluoropropionamides			
	PFPI	Pentafluoropropionamides			
	HFAA	Heptafluorobutyamides			
	HFBI	Heptafluorobutyamides			
	Alkylation	MethElute Reagent (TMPAH)	Methyl Amides	On-column derivatization for specific drugs	
<b>Carbohydrates</b> $(\text{CH}_2\text{OH})_n$	Silylation	MSTFA	TMS	Can be used with some syrups	
		TMSI	TMS		
		Tri-Sil Reagents	TMS		
	Acylation	MBTFA	Trifluoroacetates	Volatile derivatives of mono-, di- and trisaccharides	
	TFAI	Trifluoroacetates			
<b>Carboxyl</b> $\begin{array}{c} \text{O} \\    \\ \text{-C-OH} \end{array}$	Silylation	BSA	TMS	Easily formed, generally not stable, analyze quickly	
		BSTFA	TMS		
		BSTFA+TMCS	TMS		
		MSTFA	TMS		
		TMCS	TMS		Can be used with some salts
		TMSI	TMS		
		Tri-Sil Reagents	TMS		
		MTBSTFA	TBDMCS		More stable than TMS derivatives
		MTBSTFA+TBDMCS	TBDMCS		TBDMCS aids derivatization
		Alkylation	PFBBr		Pentafluorobenzyl Esters
BF <sub>3</sub> -Methanol	Methyl Esters		Best for large samples of fatty acids		
Methylate Reagent (DMFDMA)	Methyl Esters		Fatty acids and amino acids		
MethElute Reagent (TMPAH)	Methyl Esters		On-column derivatization		
PFAA+Pentafluoropropanol	Pentafluoropropyl Ester		Drug analysis		
<b>Hydroxyl-OH</b> $\text{R-OH}$ Alcohols	Silylation	BSA	TMS	Most often used derivatives	
		BSTFA	TMS		Good thermal stability
		BSTFA+TMCS	TMS		Poor hydrolytic stability
		HMDS	TMS		Weak donor usually used with TMCS
		MSTFA	TMS		
		MSTFA+TMCS	TMS		
		TMCS	TMS		Weak donor usually used with HMDS; can be used with salts
		TMSI	TMS		Can be used with syrups
		Tri-Sil Reagents	TMS		
		Phenols	MTBSTFA		TBDMCS
MTBSTFA+TBDMCS	TBDMCS		TBDMCS aids derivatization		
MBTFA	Trifluoroacetates		Good for trace analysis with EDC		
TFAA	Trifluoroacetates		Good for trace analysis with EDC		
TFAI	Trifluoroacetates		Good for trace analysis with EDC		
Phenols	PFAA	Pentafluoropropionates	Good for trace analysis with EDC		
	HFBI	Heptafluorobutyates	Good for trace analysis with EDC		
	HFAA	Heptafluorobutyates	Good for trace analysis with EDC		
	PFBBr	Pentafluorobenzyl Ethers	With alkoxides only		

## Derivatization Reagents for Drugs of Abuse

Drug	Form	Reagent		
Amphetamines 	Amphetamines	BSTFA		
	Amphetamines	HFAA		
	Amphetamines	HFAA/PFAA		
	Amphetamines	MSTFA with TMCS		
	Amphetamines	TFAA		
Methamphetamine	TFAA			
Barbiturates 		BSTFA		
		MethElute Reagent (TMPAH)		
		Methylate Reagent (DMFDMA) PFBBr		
Cocaine 	Benzoylecgonine	BSTFA/Butyl Iodine/TMPAH		
		BSTFA MTBSTFA PFAA/PFPOH		
LSD 		BSA BSTFA MSTFA TFAI		
Marijuana 	THC metabolites	BSA		
		BSTFA/BSTFA+1% TMCS		
		BSTFA/TMCS/TMSI		
		MSTFA		
		MSTFA/MSTFA+1% TMCS		
		MTBSTFA		
		PFBBr		
		PFAA/HFIOH		
		PFAA/PFPOH		
		TFAA and BF <sub>3</sub> /MeOH		
MethElute Reagent (TMPAH)				
TMSI				
Opiates 	Morphine	BSTFA+1% TMCS MBTFA PFAA TFAA BSTFA		
	Morphine/Codeine	BSTFA+1% TMCS		
		BSTFA/TFAI		
		HFBA		
		MBTFA		
		PFAA		
		PFAA/HFAA		
		PFAA/PFPOH		
		TFAA		
		Trimethylsilyl		
		PCP 	PPC/PCHP/PCP	BSTFA+1% TMCS HFAA

See references on following page.

† Reagent names correspond to product names as listed in this catalog, except PFPOH (pentafluoropropanol).

HFIOH (heptafluoro-isopropanol) is not offered by Thermo Fisher Scientific. PFAA (PentaFluoropropionic Acid Anhydride) and HFAA (HeptaFluorobutyric Acid Anhydride) are sometimes incorrectly referred to as PFPA and HFBA (respectively), which are the appropriate abbreviations for the free acid.

# Derivatization Reagents for Drugs of Abuse *continued*

## References

- Dutt, M.C. (1982). *J. Chromatogr.* **248**, 115-124.
- Wu, A.H.B., et al. (1992). *J. Anal. Toxicol.* **16**, 137-141.
- Thurman, E.M., et al. (1992). *J. Anal. Toxicol.* **16**, 19-27.
- Reimer, M.L., et al. (1993). *Biol. Mass Spectrom.* **22**, 235-242.
- Yamamoto, T., et al. (1989). *J. Anal. Toxicol.* **13**, 117-119.
- Wu, A.H.B., et al. (1992). *Biol. Mass Spectrom.* **21**, 278-284.
- Rood, H.D. and Knitter, J.A. (1991). *Capillary Chromatography*. W.G. Jennings, ed., pp. 115-130.
- DePace, A., et al. (1990). *J. Forensic Sci.* **35**(6), 1431-1435.
- Mulé, S.J. and Casella, G.A. (1998). *J. Anal. Toxicol.* **12**, 102-107.
- Suzuki, S., et al. (1983). *J. Chromatogr.* **267**, 381-387.
- Kananen, G., et al. (1972). *J. Chromatogr. Sci.* **10**, 283-287.
- Skinner, R., et al. (1973). *Anal. Chem.* **45**(3), 574-576.
- Mulé, S.J. and Casella, G.A. (1989). *J. Anal. Toxicol.* **13**, 13-16.
- Christophersen, A.S. and Rasmussen, K.E. (1980). *J. Chromatogr.* **192**, 363-374.
- Venturella, V.S., et al. (1973). *J. Pharm. Sci.* **62**(4), 662-668.
- Walle, T. (1975). *J. Chromatogr.* **114**, 345-350.
- Ellerbe, P., et al. (1992). *J. Anal. Toxicol.* **16**, 158-162.
- Graffeo, A.P., et al. (1976). *J. Chromatogr.* **126**, 712-717.
- Harkey, M.R., et al. (1991). *J. Anal. Toxicol.* **15**, 260-265.
- Bodor, G., et al. (1990). *Clin. Chem.* **36**, 742-747.
- Jane, I. and Wheals, B.B. (1973). *J. Chromatogr.* **84**, 181-186.
- Nelson, C.C. and Foltz, R.L. (1992). *Anal. Chem.* **64**, 1578-1585.
- Lim, H.K., et al. (1988). *Anal. Chem.* **60**, 1420-1425.
- Harvey, D.J. (1981). *Biomed. Mass. Spec.* **8**(8).
- Parry, R.C., et al. (1990). *J. Anal. Toxicol.* **14**, 39-43.
- Clatworthy, A.J. (1990). *Forensic Sci. Int.* **46**, 219-230.
- Baker, T.S., et al. (1984). *J. Anal. Toxicol.* **8**, 255-259.
- Clouette, R., et al. (1993). *J. Anal. Toxicol.* **17**, 1-4.
- Rosenfeld, J.M., et al. (1986). *Anal. Chem.* **58**, 716-721.
- McBurney, L.J., et al. (1986). *J. Anal. Toxicol.* **10**, 56-64.
- Karlsson, L., et al. (1983). *J. Anal. Toxicol.* **7**, 198-202.
- Foltz, R.L. (1984). *Advances in Analytical Toxicology*, I. R.C. Baselt, ed. Foster City, CA: Biomedical Publications.
- Wilkinson, G.R., et al. (1969). *Biochem. Pharmacol.* **18**, 1435-1439.
- Weitz, C.J., et al. (1986). *Proc. Nat. Acad. Sci.* **83**, 9784-9788.
- Fehn, J. and Megges, G. (1985). *J. Anal. Toxicol.* **9**, 134-138.
- Wasels, R., et al. (1989). *J. Chromatogr.* **489**, 411-418.
- Christopherson, A.S., et al. (1987). *J. Chromatogr.* **422**, 117-124.
- Chen, B.H., et al. (1990). *J. Anal. Toxicol.* **14**, 12-17.
- Bowie, L. and Kirkpatrick, P.B. (1989). *J. Anal. Toxicol.* **13**, 326-329.
- Nelson, C.C. and Foltz, R.L. (1992). *Anal. Chem.* **64**, 1578-1585.
- Grinstead, G.F. (1991). *J. Anal. Toxicol.* **15**, 293-298.
- Fuller, D.C. and Anderson, W.H. (1992). *J. Anal. Toxicol.* **16**, 315-318.
- Lee, H.M. and Lee, C.W. (1991). *J. Anal. Toxicol.* **15**, 182-187.
- Woodworth, J.R., et al. (1984). *J. Anal. Toxicol.* **8**, 2-6.
- Cone, E., et al. (1981). *J. Chromatogr.* **223**, 331-339.

## Drugs of Abuse Derivatization Applications

### Cocaine Metabolites

- Cardenas, S., et al. (1996). *Rapid Commun. Mass Spectrom.* **10**, 631-636.
- Crouch, D.J., et al. (1995). *J. Anal. Toxicol.* **19**, 352-358.
- Smimow, D., et al. (1995). Presented at the Society of Forensic Toxicologists, Baltimore, MD, 72.
- Okeke, C.C., et al. (1994). *Chromatographia* **38**, 52-56.
- Cone, E.J., et al. (1994). *Clin. Chem.* **40**, 1299-1305.
- Peterson, K.L., et al. (1994). Presented at the 46th Annual Meeting of the American Academy of Forensic Sciences, San Antonio, TX, 197.
- Moore, J.M., et al. (1993). *J. Forensic. Sci.* **38**, 1305-1325.
- Aderjan, R.E., et al. (1993). *J. Anal. Toxicol.* **17**, 51-55.
- Taylor, R.W., et al. (1991). *Adv. Lab Autom. Rob.* **7**, 567-582.
- Ortuno, J., et al. (1990). *J. Pharmaceut. Biomed. Anal.* **8**, 911-914.
- Verebey, K., et al. (1989). *J. Forensic Sci.* **34**, 46-52.
- Vasiliades, J. (1989). *J. Anal. Toxicol.* **13**, 127.
- Isenschmid, D.S., et al. (1988). *J. Anal. Toxicol.* **12**, 242-245.
- Mule, S.J., et al. (1988). *J. Anal. Toxicol.* **12**, 153-155.

### Derivatization of Cannabinoids

- Prest, H. Advantages of positive chemical ionization mass spectroscopy. Application Note. Hewlett Packard Co.
- Lisi, A.M., et al. (1993). *J. Chromatogr.* **617**, 265-270.
- Wu, A.H.B., et al. (1993). *J. Anal. Toxicol.* **17**, 215-217.
- Clouette, R., et al. (1993). *J. Anal. Toxicol.* **17**, 1-4.
- Fysh, R.R. (1989). Presented at the 26th International Meeting of the International Association of Forensic Toxicologists, Glasgow, Scotland, 67.
- Rosenfeld, J.M., et al. (1989). *Anal. Chem.* **61**, 925-928.
- Baker, T.S., et al. (1984). *J. Anal. Toxicol.* **8**, 255-259.
- Karlsson, L., et al. (1983). *J. Anal. Toxicol.* **7**, 198-202.
- Borys, H.K., et al. (1981). *J. Chromatogr.* **205**, 303-323.

### Derivatization of Amphetamines

- Kuroda, N., et al. (1998). *J. Chromatogr. A.* **798**, 325-334.
- Dasgupta, A., et al. (1998). *Amer. J. Clin. Pathol.* **109**, 527-532.
- Cheung, S., et al. (1997). *J. Chromatogr. B.* **690**, 77-87.
- Sadeghipour, F., et al. (1997). *J. Chromatogr. A.* **761**, 71-78.
- Hara, K., et al. (1997). *J. Anal. Toxicol.* **21**, 54-58.
- Shin, H.-S., et al. (1996). *Anal. Chem.* **68**, 3015-3020.
- Meatherall, R.C. (1994). Presented at the 1994 TIAFT-SOFT Program, Tampa, FL, 66.
- Thompson, W.C., et al. (1994). *Clin. Chem.* **40**, 1703-1706.
- Sievert, H.J.P. (1994). *Chirality* **6**, 295-301.
- Melgar, R., et al. (1993). *J. Anal. Toxicol.* **17**, 399-402.
- Jones, J.B., et al. (1993). *J. Anal. Toxicol.* **17**, 447.
- Gjerde, H., et al. (1993). *J. Anal. Toxicol.* **17**, 65-68.
- Cody, J.T., et al. (1992). *J. Chromatogr.* **580**, 77-95.
- Hughes, R.O., et al. (1991). *J. Anal. Toxicol.* **15**, 256-259.
- Gan, B.K., et al. (1991). *J. Forensic Sci.* **36**, 1331-1341.
- Lillsunde, P., et al. (1991). *Forensic Sci. Int.* **49**, 205-213.
- Rasmussen, S., et al. (1989). *J. Anal. Toxicol.* **13**, 263-267.
- Czarny, R.J., et al. (1989). *J. Anal. Toxicol.* **13**, 257-262.
- Hornbeck, C.L., et al. (1989). *J. Anal. Toxicol.* **13**, 144-149.

### Derivatization of Opiates

- Brendler, J.P., et al. (1998). Presented at the AAFS, San Francisco, CA.
- Balikova, M., et al. (1998). *Forensic Sci. Int.* **94**, 201-209.
- Emara, S. (1998). *Biomed. Chromatogr.* **12**, 15-20.
- Hyytynen, T., et al. (1997). *J. Chromatogr. A.* **771**, 360-365.
- Guillot, J.G., et al. (1997). *J. Anal. Toxicol.* **21**, 127-133.
- Dietzen, D.J., et al. (1995). *J. Anal. Toxicol.* **19**, 299-303.
- Hendrickson, T.L., et al. (1994). *J. Chromatogr. B.* **653**, 147-154.
- Nakahara, Y., et al. (1992). *Arch. Toxicol.* **66**, 669-674.
- Chari, G., et al. (1991). *J. Chromatogr.* **571**, 263-270.
- Lee, H.-M., et al. (1991). *J. Anal. Toxicol.* **15**, 182-187.
- Chen, B.H., et al. (1990). *J. Anal. Toxicol.* **14**, 12-17.
- McLean, C.F., et al. (1990). *J. Pharm. Pharmacol.* **42**, 669-671.
- Wasels, R., et al. (1989). *J. Chromatogr.* **489**, 411-418.
- Battah, A.-K., et al. (1989). Presented at the 26th Annual International Meeting of the International Association of Forensic Toxicologists, Glasgow, Scotland, 16.
- Derks, H.J.G.M., et al. (1986). *J. Chromatogr.* **370**, 173-178.
- Moore, J.M., et al. (1984). *Anal. Chem.* **56**, 642-646.

## Troubleshooting Reagents

Derivatization Problem	Possible Cause	Recommended Solution
Low Yield	Carrier, air, detector (FID) hydrogen or make-up gas flow set incorrectly	Measure flows using a Thermo Scientific GFM Pro Gas Flow Meter and set accordingly using instrument manufacturer's recommendations
	Reagent deteriorated	Store reagent properly to prevent oxygen/water contamination, temperature damage (refer to product specification sheet)
	Rate of reaction too slow	Re-evaluate reagent concentration, time, temperature and consider heating the reaction mix (consider the thermal stability of the analytes and reagents)
	Water in reaction mix	Remove water by adding sodium sulfate to sample. Store reagent properly to prevent oxygen/water contamination
	Improper handling technique: (e.g. Low boiling components could be lost during sample concentration); sample too dilute; wrong solvent	Re-evaluate technique, if possible eliminate steps in which analyte could be adsorbed or otherwise lost (unnecessary transfers etc.)
	Wrong reagent	Re-evaluate reagent selection and select more appropriate reagent
	Impurities in solvent, starting material, catalysts, or extract interfering with derivatization (e.g. Plasticizers from vial, inorganics used in sample synthesis, preservatives or antioxidants in solvents)	Use only highest purity material at all steps in the sample preparation process
	Reagent: sample ratio too low	Use more reagent for same amount of sample
	Sample adsorbed to glassware	Deactivate glassware, inlet sleeve and column by silanizing
No sample separation after adding reagent and heating	Septum in reaction vial not sealed	Prepare a new sample and derivatize. Be sure that the vial is sealed
Detector response low	Sample components absorbed by inlet liner or column	Inject standard on column known to be performing well. If results are good, remove inlet liner and check cleanliness. Use new, deactivated liner or replace glass wool and packing. Rinse bonded phase column or remove a few cm from inlet end of non-bonded column. If performance is not restored, replace column
	Low yield of derivative – reaction did not go to completion	Add more reagent, increase temperature or heating time or add catalyst. Water may be present; add sodium sulfate to sample
	Detector (FID) dirty	Clean FID as per instrument manual
Extra peak(s)	Derivative reacting with solvent	Use a solvent that does not have an active hydrogen, alcohol or enolizable ketone group (e.g. Hexane, toluene etc.)
	Impurities from sample solvent, reagents, sample vial, other labware	Inject solvent and reagents blanks, solvent rinse from unused vial etc. Isolate sources of impurities
	Reagents interacting with column	Verify that reagent is compatible with analytical column
	Derivative undergoing hydrolysis	Remove water by adding sodium sulfate to sample. Store reagent properly to prevent oxygen/water contamination
Missing peaks or solvent peak only	Wrong reagent	Re-evaluate reagent selection
	Reagent deteriorated	Store reagent properly to prevent oxygen/water contamination, temperature damage (refer to product specification sheet)
	Rate of reaction too slow	Re-evaluate reagent concentration, time, temperature and consider heating the reaction mix (consider the thermal stability of the analytes and reagents)
	Impurities in solvent, starting material, catalysts, or extract interfering with derivatization (e.g. Plasticizers from vial, inorganics used in sample synthesis, preservatives or antioxidants in solvents)	Use only highest purity material at all steps in the sample preparation process
	Sample adsorbed to glassware	Deactivate glassware, inlet sleeve and column by silanizing
	Reagent: sample ratio too low	Use more reagent for same amount of sample
	Water in reaction mix	Remove water by adding sodium sulfate to sample. Store reagent properly to prevent oxygen/water contamination

# Resources

for Chromatographers



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