JEOL

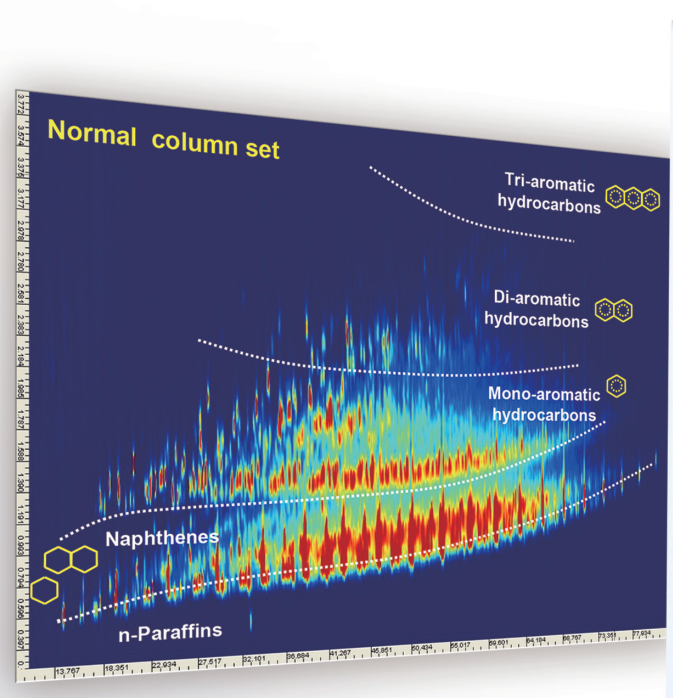
Scientific / Metrology Instruments

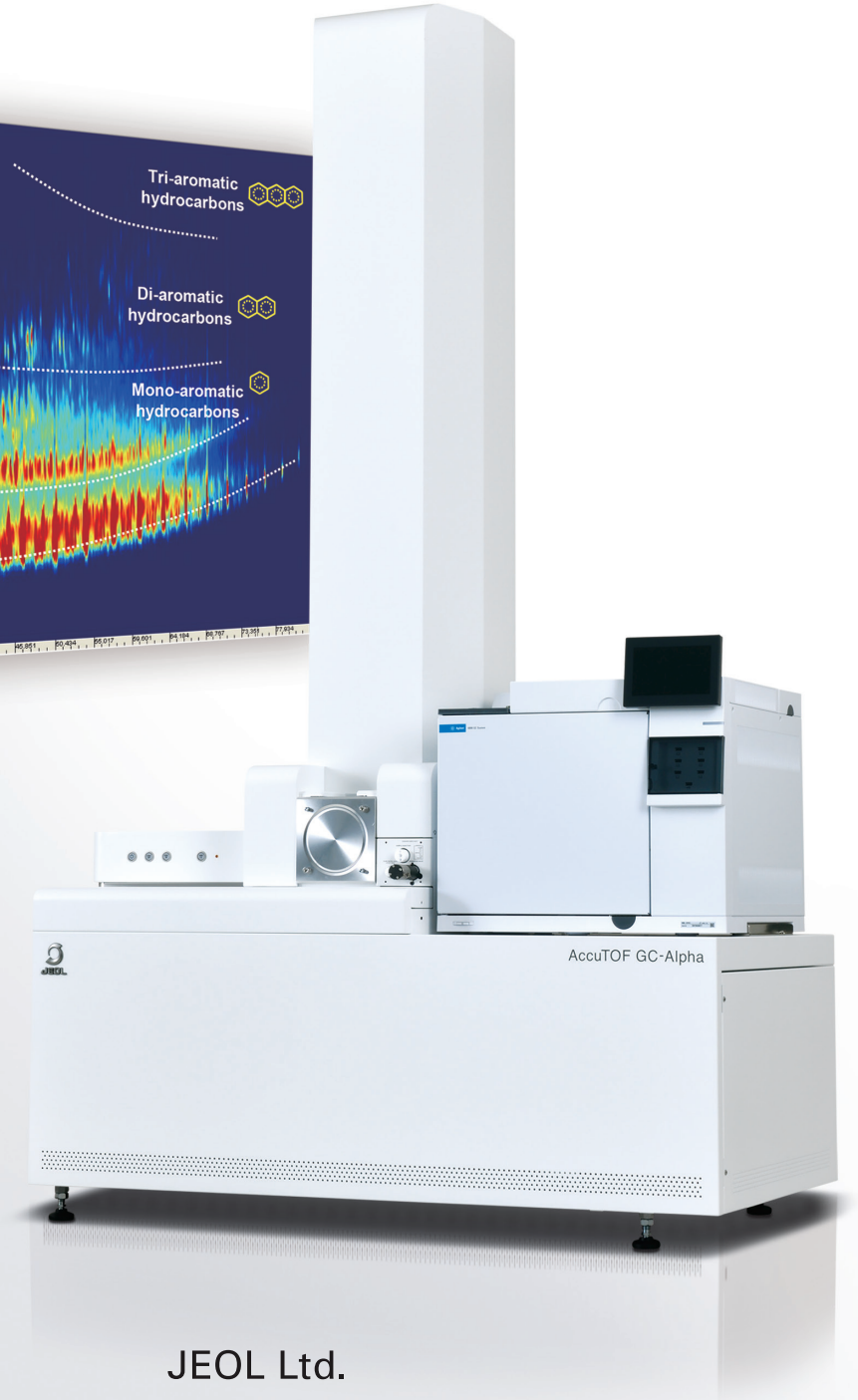
High Performance Gas Chromatograph – Time-of-Flight Mass Spectrometer

Solutions for Innovation

JMS-T2000GC AccuTOF™ GC-Alpha

Petroleum and Petrochemical Solutions





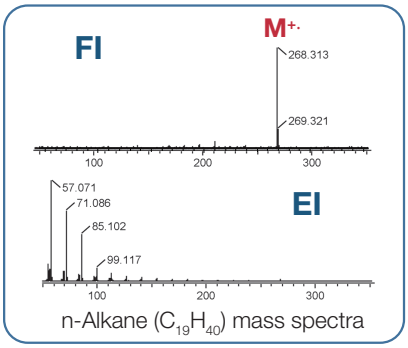
JEOL Ltd.

High Resolution, Time-of-Flight Mass Spectrometer

High mass-resolution, which enables differentiation of various classes of hydrocarbons by their exact masses, in combination with soft ionization methods, which enable unambiguous detection of hydrocarbon molecular ions, is an extremely powerful tool for petroleum and petrochemical analyses.
The JMS-T2000GC AccuTOF™ GC-Alpha is a superior gas chromatograph – high-resolution time-of-flight mass spectrometer (GC-HRTOFMS) system that simultaneously accomplishes high mass-resolution analysis, high mass accuracy, and high-speed data acquisition, satisfying all your needs for petroleum and petrochemical analyses.
The JMS-T2000GC AccuTOF™ GC-Alpha is the 6th generation of the successful AccuTOF™ GC series of instruments. Since the introduction of the 1st generation JMS-T100GC AccuTOF™ GC in 2004, we have installed more than 270 AccuTOF™ GC series of instruments around the world*, making the AccuTOF™ GC series the most popular GC-HRTOFMS.
* As of April 2021

Softest Ionization for Petroleum Samples

Field Ionization (FI) and Field Desorption (FD) are well suited for hydrocarbons analysis because they generate molecular ions for almost all compounds, including saturated hydrocarbons, with minimal fragmentation. The ionization process for these techniques is carried out in a high-potential electric field (~10^8 V/cm) that is made between a FI/FD emitter (Anode) and a counter electrode (Cathode). A molecular ion is created within the high-potential electric field by electron tunneling between the analyte molecules and the emitter. The resulting mass spectra are dominated by molecular ions, whether from the GC output (FI) or from the emitter surface (FD).



n-Alkane ($C_{19}H_{40}$) mass spectra

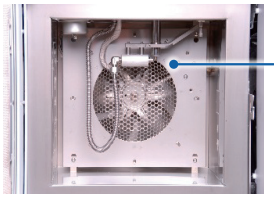
Two Optional Combination Ion Sources: EI/FI/FD and EI/PI

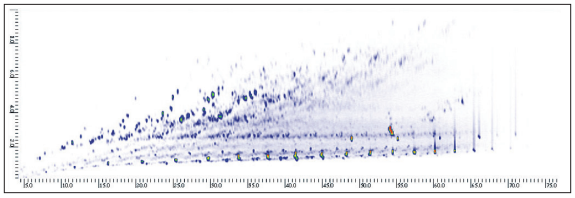
The EI/FI/FD combination ion source is a unique accessory that is only offered on the JEOL AccuTOF™ GC-Alpha system. EI and FI/FD modes can be switched by simply exchang-ing the EI repeller probe and the FI/FD emitter probe, without breaking vacuum. As a result, both GC/EI (or GCxGC/EI; see below) and GC/FI (or GCxGC/FI) measurements can be done (along with FD) using a single ion source.
Additionally, JEOL offers an EI/Photoionization (PI) combination ion source for the AccuTOF™ GC-Alpha. While FI is still the softest ionization technique available, PI can also be used to generate molecular ions for many analytes, including hydrocarbons. In particular, aromatic hydrocarbons, which strongly absorb UV light, are preferentially ionized with PI, making the technique useful for detecting aromatic hydrocarbons in complex mixtures. In this case, each method is available by turning on the filament for EI or the UV lamp for PI. As a result, both GC/EI (or GCxGC EI) and GC/PI (or GCxGC/PI) measurements can also be done using a single ion source.

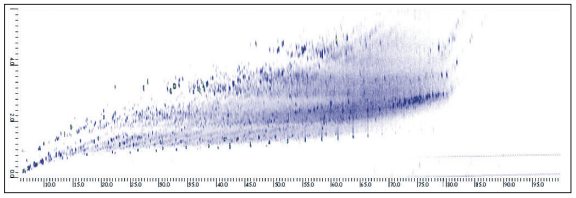
Note: use of an EI/FI/FD combination ion source or an EI/PI combination ion source as a substitute of a standard EI ion source for routine analyses is not recommended.

Comprehensive Two-dimensional GC Technique

Comprehensive two-dimensional gas chromatography (GCxGC) consists of two different types of columns that are connected via a thermal modulator (Zoex Co.) within the same GC oven. The GCxGC system requires a fast-acquisition detection system to allow for the detection of peaks with very narrow widths in the 2D GC chromatograms. The AccuTOF™ GC-Alpha has a high-speed data acquisition capability with a spectral acquisition rate of up to 50 Hz (0.02sec/spectrum). Therefore, the AccuTOF™ GC-Alpha system can be successfully used as a GCxGC detector.


Zoex thermal modulator inside GC oven


GCxGC/FI TICC for a diesel fuel


GCxGC/FI TICC for a crude oil

Note: Zoex's GCxGC system is provided and supported through Zoex's sales and support network and may not be available in your territory. Contact your local JEOL representative for detail.

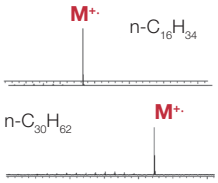
GCxGC/FI Type Analysis

Comprehensive two-dimensional gas chromatography (GCxGC) in combination with high-resolution mass spectrometry (HRMS) is a powerful tool for the analysis of complex mixtures. Field ionization (FI) is a soft ionization technique that is well suited for hydrocarbons analysis because it generates molecular ions for almost all compounds with minimal fragmentation. We can get individual hydrocarbon information (formula, carbon number, intensity) easily from molecular ions which are generated by FI. We do not need to use complex EI fragmentation information to carry out type analysis. There are several advantages of GCxGC/FI-HRMS method for detailed type analysis of petroleum samples.

1. FI is ideal for hydrocarbon compounds because it generates abundant molecular ions.
2. High selectivity (with narrow *m/z* windows) allows high-precision extracted ion chromatograms.
3. GCxGC provides exceptional separation capacity with 2D structure-retention relationships.

FI is Ideal for Hydrocarbon Compounds

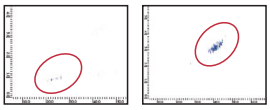
FI can generate molecular ions with minimal fragmentation, thus making them easily identifiable for all hydrocarbons.



FI mass spectra of n-Alkanes

High selectivity Extracted Ion Chromatogram (EIC)

High mass resolution can provide high selectivity (narrow *m/z* window) for the EIC. Hydrocarbon peaks that have the same nominal mass, but different exact mass, can be separated completely.

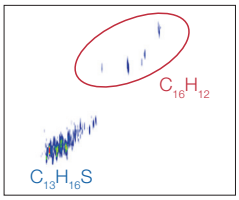


GCxGC/FI EIC of *m/z* 184.2192 ($C_{13}H_{28}$)

GCxGC/FI EIC of *m/z* 184.1253 ($C_{14}H_{16}$)

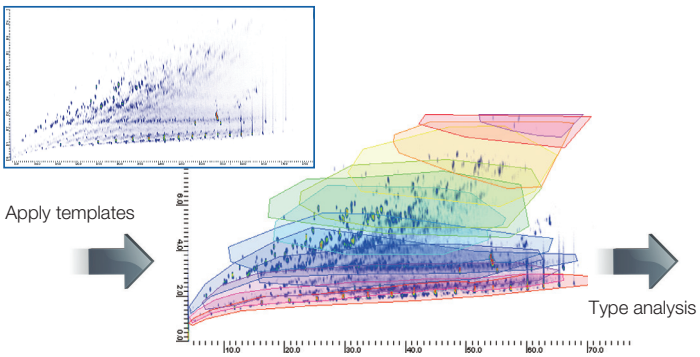
GCxGC Provides Exceptional Separation

The AccuTOF™ GC-Alpha has high mass resolution capability, but for some components, mass separation can be difficult. For example, the separation between PAHs ($C_{16}H_{12}$, *m/z* 204.0939) and Benzothiophenes ($C_{13}H_{16}S$, *m/z* 204.0973) would require over 180,000 mass resolving power to separate by mass alone. However, GCxGC separates these compound classes by chromatography, so ultrahigh resolving power is not necessary to correctly assign and quantify these compounds.

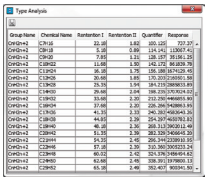


GCxGC/FI EIC of *m/z* 204.0939

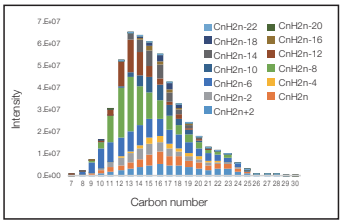
Templates for various hydrocarbon series can be created within GC Image (GC Image, LLC) GCxGC/MS data processing software. Then the templates can be applied to any hydrocarbon data acquired with the same GCxGC conditions.



Type analysis templates of 13 hydrocarbon series:
C_nH_{2n+2}, C_nH_{2n}, C_nH_{2n-2}, C_nH_{2n-4}, C_nH_{2n-6}, C_nH_{2n-8}, C_nH_{2n-10}, C_nH_{2n-12}, C_nH_{2n-14}, C_nH_{2n-16}, C_nH_{2n-18}, C_nH_{2n-20} and C_nH_{2n-22}

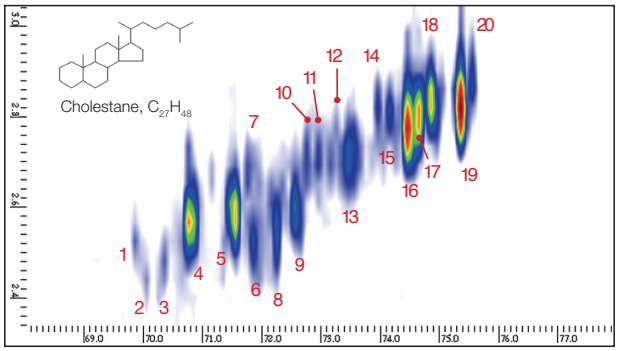


Export to MS Excel

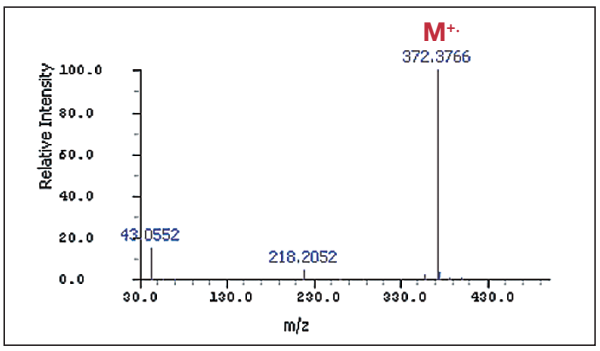


Biomarker Analysis

Fragment ions from electron ionization (EI) can cause interferences for biomarker detection. For example, fragments resulting from loss of a methyl group have isotope peaks that can be confused with molecular ions from related compounds. FI solves this problem because it does not produce the fragment ions. We clearly identified 20 isomers of cholestane $C_{27}H_{48}$ in a crude oil sample by GCxGC/FI. The GCxGC/FI extracted ion chromatograms made it easy to interpret the data and correctly assign the biomarker peaks.



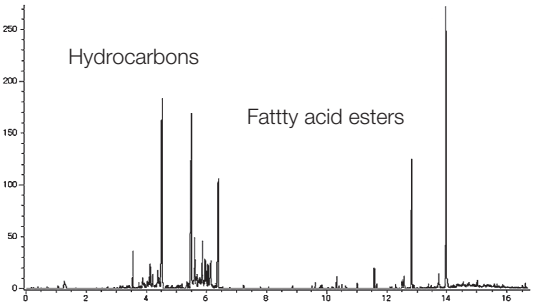
GCxGC/FI EIC for $C_{27}H_{48}$ molecular ion in a crude oil



FI mass spectrum of #16

One-dimensional GC/FI

Regular one-dimensional GC/FI measurements are easily carried out using the AccuTOF™ GC-Alpha. In addition to normal-speed GC/FI measure-ments, this system is also capable of doing fast GC measurements, which use short (5-10 m), narrow bore (0.1-0.15 mm I.D.) capillary columns. This fast GC/FI technique allows for the quick determination of molecular ion information for a wide variety of the samples.



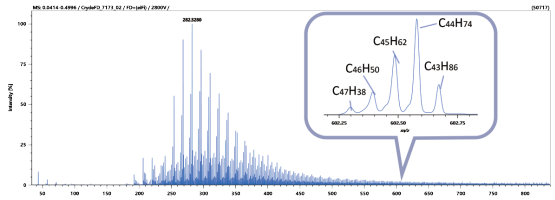
GC/FI TICC for a lubricant oil

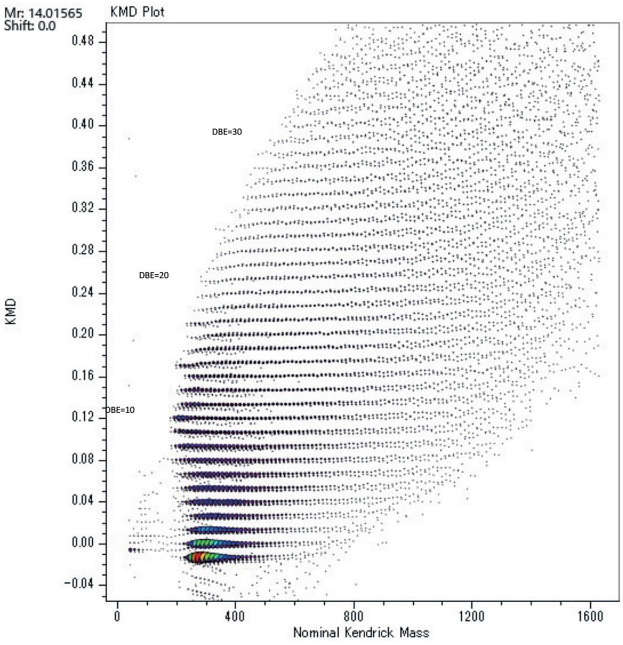
Analysis of Crude Oil with FD and msRepeatFinder software

Using the direct inlet FD technique, crude oil that contains high boiling point components can be analyzed.
The msRepeatFinder repeating structure analysis software visualizes a complex mass spectrum as a KMD (Kendrick mass defect) plot. The KMD plot of the FD mass spectrum of the crude oil shows that the isobaric components up to 1,000 Da and DBE (double bond equivalent) up to 30 are clearly resolved with the high mass-resolving power of the AccuTOF™ GC-Alpha. By visualizing hydrocarbons of different degree of unsaturation, analysis and grouping of each series becomes an easy task.
Moreover, by grouping each series, a type analysis calculation can automatically be performed for each group that includes:

- ▶ Sum of Intensities
- ▶ Number Average Molecular Weight
- ▶ Weight Average Molecular Weight

Detailed type analysis is possible by visualizing spectra with KMD plots.





No.	Formura	DBE	Sum of Intensities	Weighted Average of KMD	Weighted Average of NKM	Number Average of molecular weitht(Mn)	Weight Average of molecular weitht(Mw)	Poly dispersity
1	C_nH_{2n+2}	0	2135838	-0.013	309.9	310.2	318.7	1.03
2	C_nH_{2n}	1	1627964	0.001	333.9	334.2	349.6	1.05
3	C_nH_{2n-2}	2	1070976	0.014	351.4	351.8	371.5	1.06
4	C_nH_{2n-4}	3	677938	0.027	376.5	376.5	401.3	1.07
5	C_nH_{2n-6}	4	943169	0.041	380.0	380.0	412.4	1.09
6	C_nH_{2n-8}	5	870604	0.054	391.2	391.2	429.7	1.10
7	C_nH_{2n-10}	6	706070	0.067	410.3	410.3	456.5	1.11
8	C_nH_{2n-12}	7	694475	0.081	410.2	410.2	466.4	1.14
9	C_nH_{2n-14}	8	764486	0.094	403.4	403.4	473.3	1.17
10	C_nH_{2n-16}	9	710217	0.108	388.7	388.7	449.2	1.16

Powerful Tools for Analysis

The JMS-T2000GC AccuTOF™ GC-Alpha provides powerful tools for the analysis of petroleum and related products. The system provides high-resolution, exact mass data for classical GC/MS analysis with electron ionization. Soft ionization methods are available as options, including chemical ionization (CI) and electron capture negative-ion analysis (ECNI), field ionization (FI), field desorption (FD), and photoionization (PI). All of these methods can be combined with comprehensive two-dimensional gas chromatography (GCxGC) to provide powerful capabilities for complex mixture analysis.

*Specifications subject to change without prior notice.

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JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
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• **AUSTRALIA & NEW ZEALAND** /JEOL (AUSTRALASIA) Pty.Ltd. Suite 1, L2 18 Aquatic Drive - Frenchs Forest NSW 2086 Australia • **BELGIUM** /JEOL (EUROPE) B.V. Planet II, Gebouw B Leuvensesteenweg 542, B-1930 Zaventem Belgium • **BRAZIL** /JEOL Brasil Instrumentos Cientificos Ltda. Av. Jabaquara, 2958 5° andar conjunto 52 ; 04046-500 Sao Paulo, SP Brazil • **CANADA** /JEOL CANADA, INC. 3275 1ere Rue, Local #8 St-Hubert, QC J3Y-8Y6, Canada • **CHINA** /JEOL (BEIJING) CO., LTD. Zhongkeziyuan Building South Tower 2F, Zhongguancun Nansanjie Street No. 6, Haidian District, Beijing, P.R.China • **EGYPT** /JEOL SERVICE BUREAU 3rd Fl. Nile Center Bldg., Nawal Street, Dokki, (Cairo), Egypt • **FRANCE** /JEOL (EUROPE) SAS Espace Claude Monet, 1 Allee de Giverny 78290, Croissy-sur-Seine, France • **GERMANY** /JEOL (GERMANY) GmbH Gute Aenger 30 85356 Freising, Germany • **GREAT BRITAIN & IRELAND** /JEOL (U.K.) LTD. JEOL House, Silver Court, Watchmead, Welwyn Garden City, Herts AL7 1LT, U.K. • **INDIA** /JEOL INDIA PVT. LTD, Unit No.305, 3rd Floor, ABW Elegance Tower, Jasola District Centre, New Delhi 110 025, India /JEOL INDIA PVT. LTD, Hyderabad Office 422, Regus Solitaire Business centre, 1-10-39 to 44, level 4, Gumidelli Towers, Old Airport Road, Begumpet, Hyderabad - 500016, India • **ITALY** /JEOL (ITALIA) S.p.A. Palazzo Pacinotti - Milano 3 City, Via Ludovico il Moro, 6/A 20079 Basiglio(MI) Italy • **KOREA** /JEOL KOREA LTD. Dongwoo Bldg. 7F, 1443, Yangjae Daero, Gangdong-Gu, Seoul, 05355, Korea • **MALAYSIA** /JEOL (MALAYSIA) SDN.BHD. 508, Block A, Level 5, Kelana Business Center, 97, Jalan SS 7/2, Kelana Jaya, 47301 Petaling Jaya, Selangor, Malaysia • **MEXICO** /JEOL DE MEXICO S.A, DE C.V. Arkansas 11 Piso 2 Colonia Napoles Delegacion Benito Juarez, C.P. 03810 Mexico D.F., Mexico • **QATAR** /Mannai Trading Company W.L.L. ALI Emadi Complex, Salwa Road P.O.Box 76, Doha, Qatar • **RUSSIA** /JEOL (RUS) LLC Office 351,.floor 3, 23, Novoslobodskaya St, Moscow 127055, Russia • **SCANDINAVIA** /SWEDEN JEOL (Nordic) AB Hammarbacken 6A, Box 716, 191 27 Sollentuna Sweden • **SINGAPORE** /JEOL ASIA PTE.LTD. 2 Corporation Road #01-12 Corporation Place Singapore 618494 • **TAIWAN** /JIE DONG CO., LTD. 7F, 112, Chung Hsiao East Road, Section 1, Taipei, Taiwan 10023 (R.O.C.) • **THE NETHERLANDS** /JEOL (EUROPE) B.V. Lireweg 4, NL-2153 PH Nieuw-Vennep, The Netherlands • **USA** /JEOL USA, INC. 11 Dearborn Road, Peabody, MA 01960, U.S.A.

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