

12039

REQUEST FOR SAMPLE ANALYSIS
Mass Spectrometry Core of the Research Technology Support Facility, Michigan State University
603 Wilson Road – Biochemistry Room 11, East Lansing, MI 48824-1319
<http://rtsf.msu.edu/massspec.html>

Please Print

Sample submitted by: Jesse Traub
Faculty Project Leader (PI): Wayne Loesch
Department: Horticulture
Shipping Address: _____
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E-mail address: traubjes@msu.edu / loesch@msu.edu
GLBRC – please provide project number: _____

For non MSU-clients: Institution/Company: _____

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Account/PO #: RC064178, sub L0E5

Please FAX a copy of PO to 517-353-6342

☐ Credit card payment (provide information on a separate sheet; will be used for this requisition only) http://rtsf.msu.edu/about_admin.html

PLEASE PROVIDE THE INFORMATION REQUESTED BELOW. SUCCESSFUL ANALYSES OF YOUR SAMPLES DEPEND UPON IT.

Please draw or attach the chemical structure. Molecular mass: _____ Elemental formula: _____

12 samples for derivitization and analysis on GC/MS.

Instrument Used: ☐ Agilent GC/MS ☐ Quattro Premier XE LC/MS/MS ☐ Xevo TQ-S LC/MS/MS ☐ Shimadzu Axima MALDI-TOF
☐ Thermo DSQ-II GC/MS ☐ Quattro micro LC/MS/MS ☐ LCQ Deca XP+ LC/MS/MS ☐ _____
☐ GCT Premier GC/TOF MS ☐ QTRAP 3200 LC/MS/MS ☐ Xevo G2-S QToF LC/MS/MS ☐ _____

☐ Solid sample. Amount provided: _____ Suitable solvent(s): _____

☐ Solution sample. Solvent used: _____ Analyte concentration: _____

☐ Special storage and handling (temperature, air/light sensitive?): _____

☐ Safety considerations (Radioactive, hazardous?): _____

Sample history (purification, preparation, reagents, buffers, detergents, other compounds present): _____

Requested Analysis

Ionization method: ☐ 70 eV EI ☐ CI ☐ APCI ☐ APPI ☐ ESI (electrospray) ☐ MALDI Polarity: ☐ (+) ☐ (-)

☐ MS/MS ☐ Product/daughter scan ☐ Precursor/parent scan ☐ Neutral loss scan for mass: _____

☐ High resolution/accurate mass on m/z _____ Anticipated ion formula: _____

☒ GC/MS ☐ LC/MS ☐ LC/MS/MS ☐ Direct probe ☐ Flow injection analysis ☐ Infusion ☐ Other _____

Column, temperature, mobile phase, gradient, other: _____

Special requests (sample/data processing): derivatization

Please acknowledge the MSU Mass Spectrometry Core in your publications

Date: Nov 7, 2012 Signature: [Signature]

Code	Service	Qty	Rate	Amount

To be completed by Facility staff: Date completed: _____ Operator: _____

Data file: _____ Time (hr): _____

Probe/FIA/Infusion: _____

Column: _____ Mass Range: _____

Program/Gradient: _____ Matrix: _____

High resolution result: _____ Ionization Mode: _____

Comments: _____

Sample Analysis #: 12039
Sample Submitted by: Jesse Traub
Analyst: Scott A. Smith, PhD

SAMPLE PREPARATION

Twelve samples were submitted as solids deposited at the bottom of Parafilm-sealed test tubes. The samples were named as follows:

- | | | | |
|-------------|------------|---------|-----------|
| 1. 1JT beta | 4. 2JT CHO | 7. WT8 | 10. T18-3 |
| 2. 3JT beta | 5. 4JT CHO | 8. WT16 | 11. T51-1 |
| 3. 6JT beta | 6. 5JT CHO | 9. WT25 | 12. T51-2 |

Microgram-level quantities of material were scraped out of each test tube using disposable polypropylene autopipettor tips. Each quantity of sample material was placed into a 2 mL polypropylene centrifuge tube. To each sample was added 50 μ L of MSTFA. All samples were then capped and subjected to a 1 hr immersion in an ultrasonic bath prior to being allowed to react at room temperature overnight. The next day, each sample was transferred into 250 μ L glass microinserts within 2 mL glass autosampler vials. An MSTFA blank was also prepared. All samples were capped with PTFE/rubber septa.

INSTRUMENT OPERATION

Samples were analyzed on an Agilent 6890N GC coupled to an Agilent 5973 *inert* mass spectrometer. A DB-5MS capillary column was installed in the GC (30 m length x 0.250 mm ID x 0.25 μ m film thickness). The inlet temperature was 250 $^{\circ}$ C, the He carrier flow rate was 1.2 mL/min, the m/z range was 30-600, and the oven ramp was as follows: 50 $^{\circ}$ C (hold for 1 minute), then 10 $^{\circ}$ C/min to 320 $^{\circ}$ C (hold for 2 minutes). All samples were analyzed with a splitless or/and a 10x split injection.

DATA SUMMARY

Total ion chromatograms for the samples and blanks may be viewed in **Figures 1-14**. Additionally, Agilent Chemstation automated peak identification lists have been generated (**Tables 1-14**); the automated peak ID program is based on a Probability Based Match (PBM) algorithm which attempts to match the mass spectrum of a given component with those available in the NIST 2005 mass spectral database. The probable reliability of a match is reflected in the PBM score for a given compound identification; the higher the PBM score, the greater is the likelihood that the program has identified the compound correctly; as a rule of thumb, PBM scores >80 are often matches with compounds that are structurally related if not an exact match.

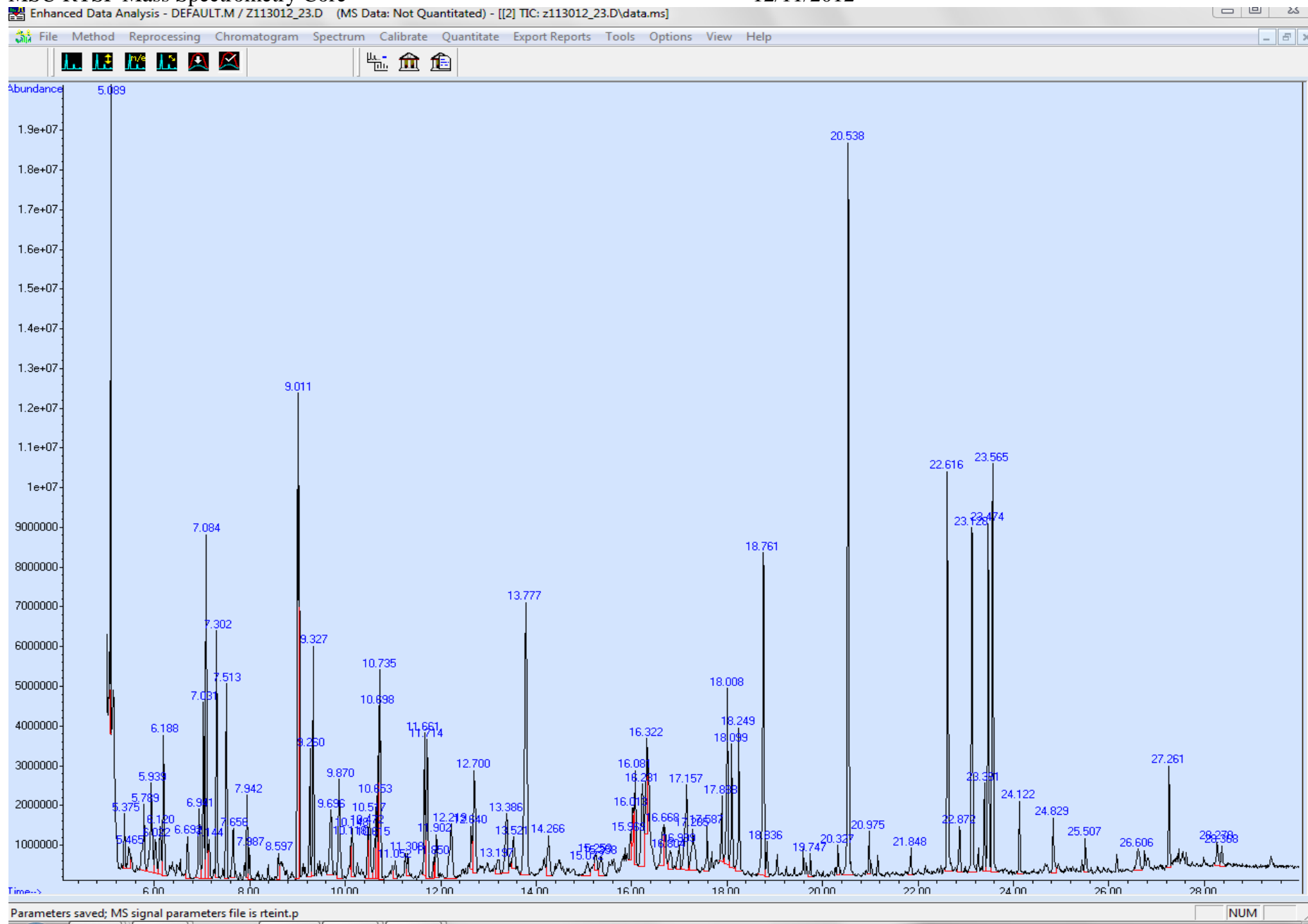


Figure 1. Total Ion Chromatogram of the sample 1JT beta. Splitless injection. File: z113012_23.

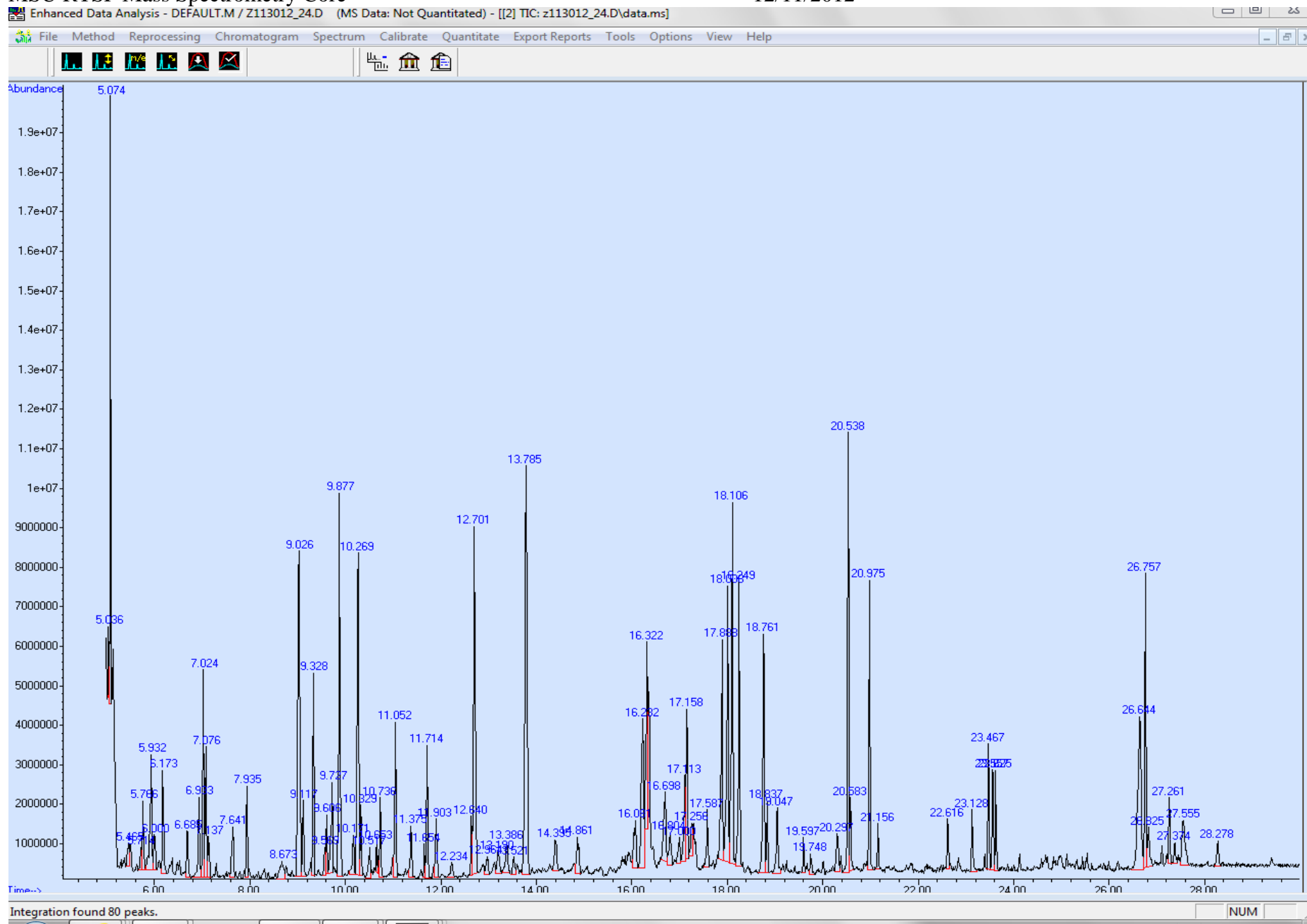


Figure 2. Total Ion Chromatogram of the sample 3JT beta. Splitless injection. File: z113012_24.



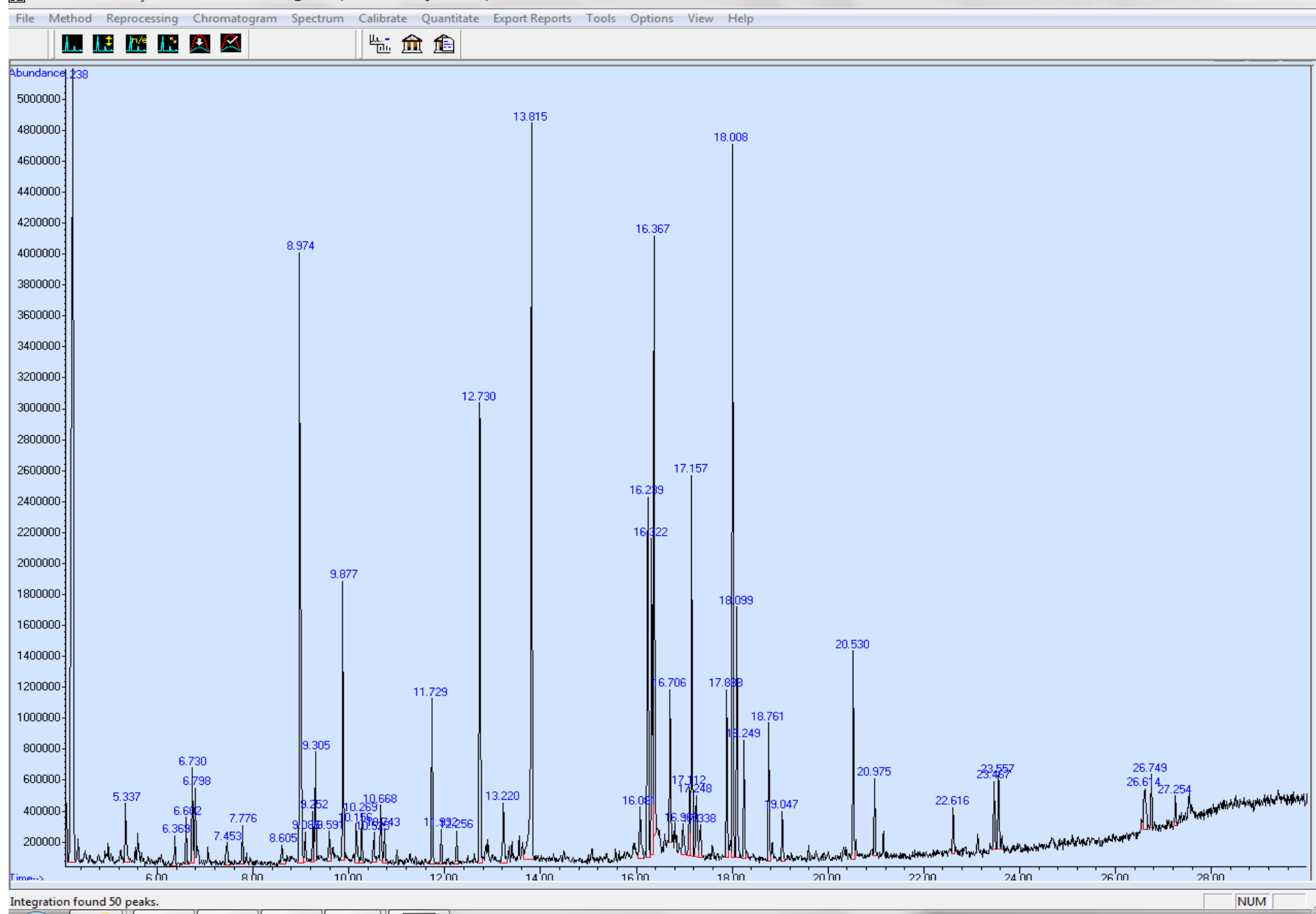


Figure 4. Total Ion Chromatogram of the sample 2JT CHO. 10x split injection. File: z113012_17.

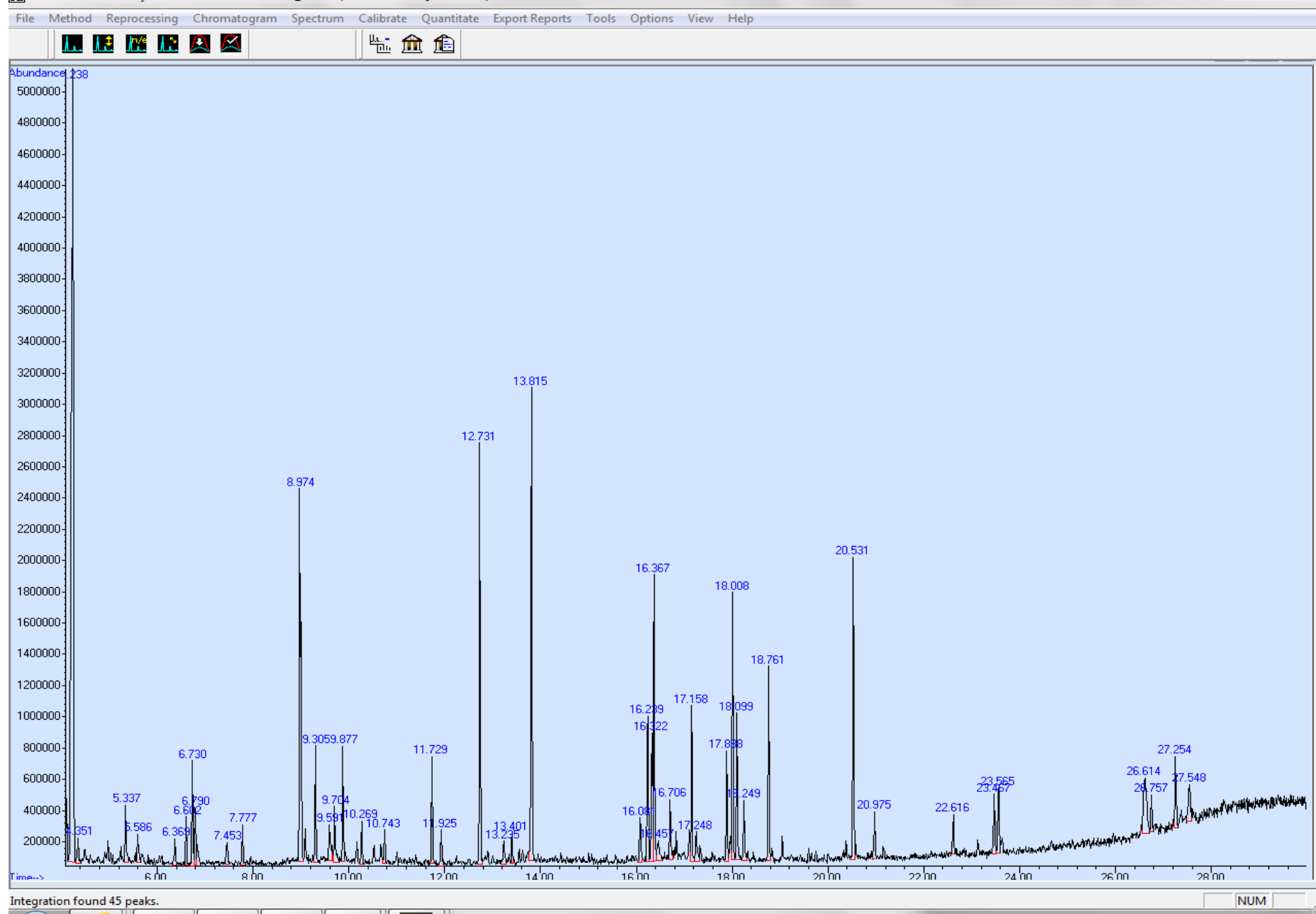


Figure 5. Total Ion Chromatogram of the sample 4JT CHO. 10x split injection. File: z113012_18.

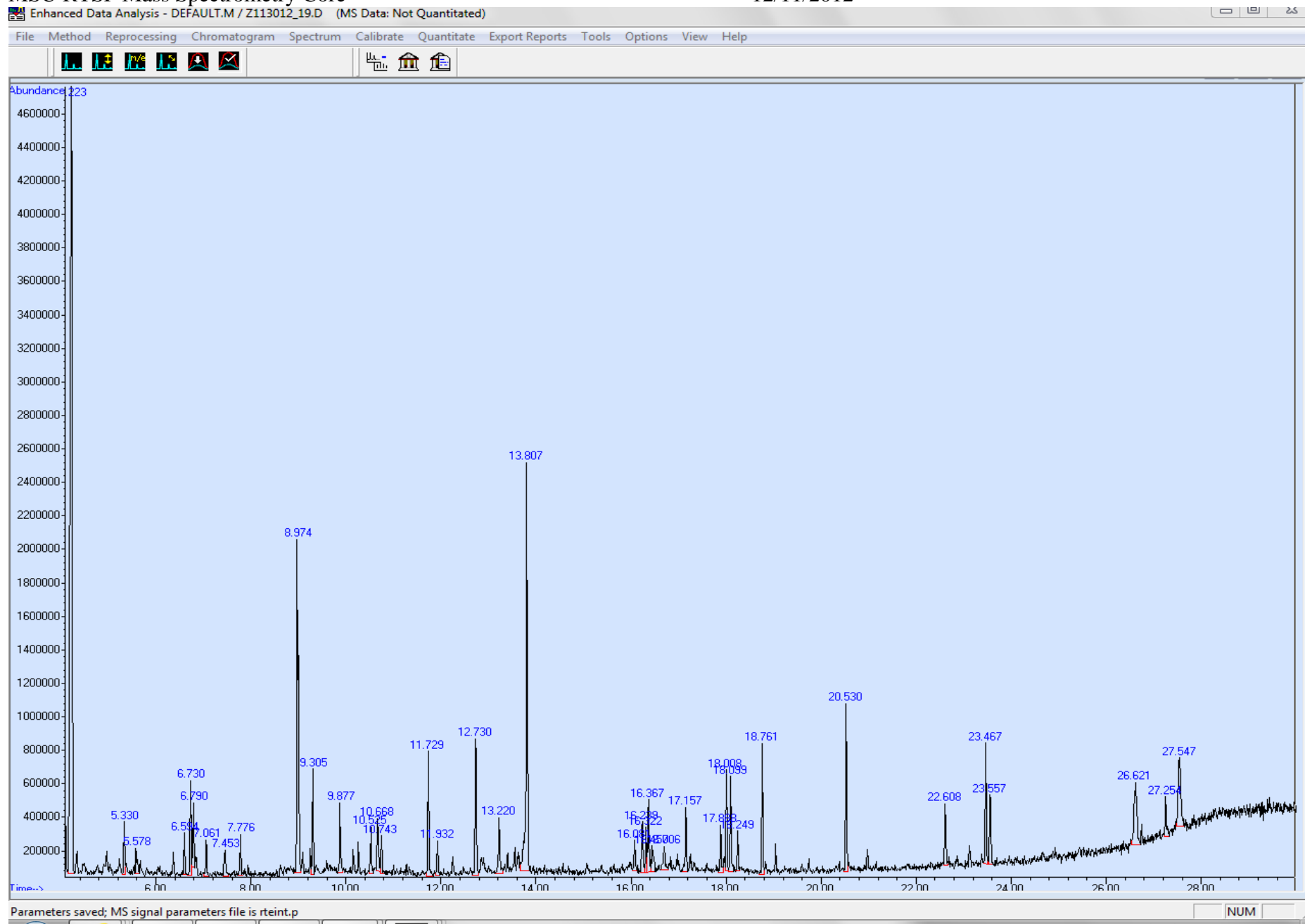


Figure 6. Total Ion Chromatogram of the sample 5JT CHO. 10x split injection. File: z113012_19.

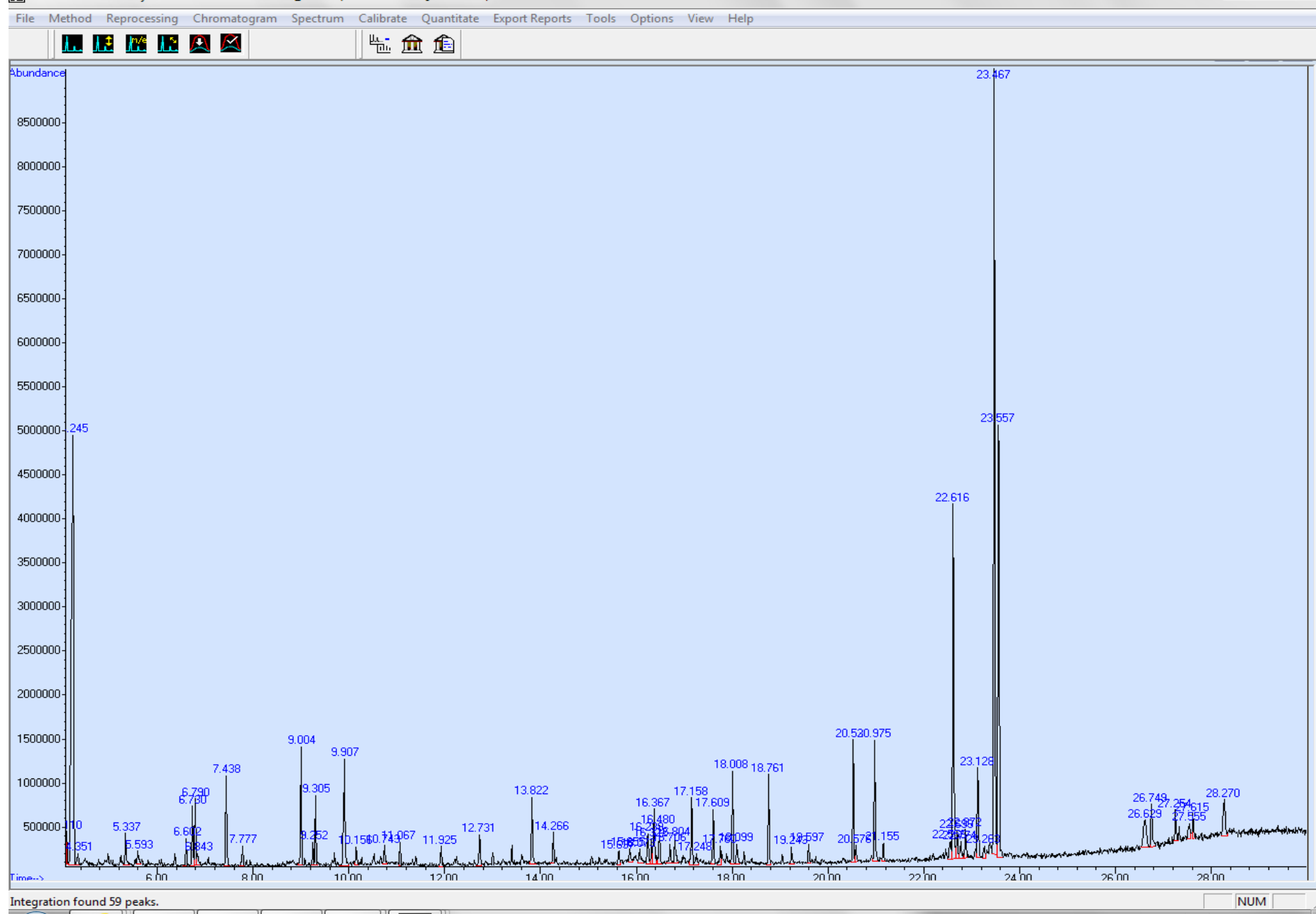


Figure 7. Total Ion Chromatogram of the sample WT8. 10x split injection. File: z113012_20.

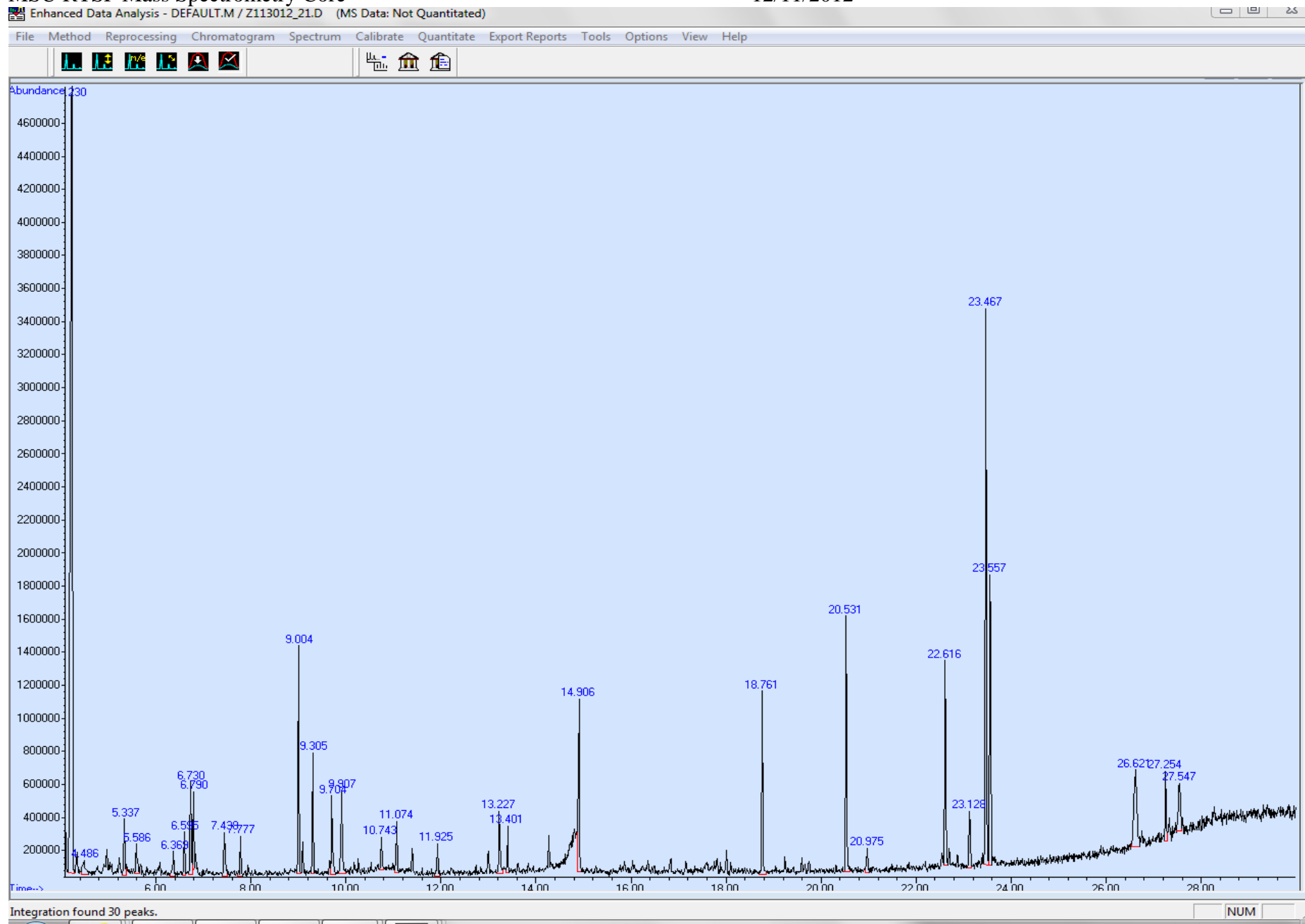


Figure 8. Total Ion Chromatogram of the sample WT16. 10x split injection. File: z113012_21.

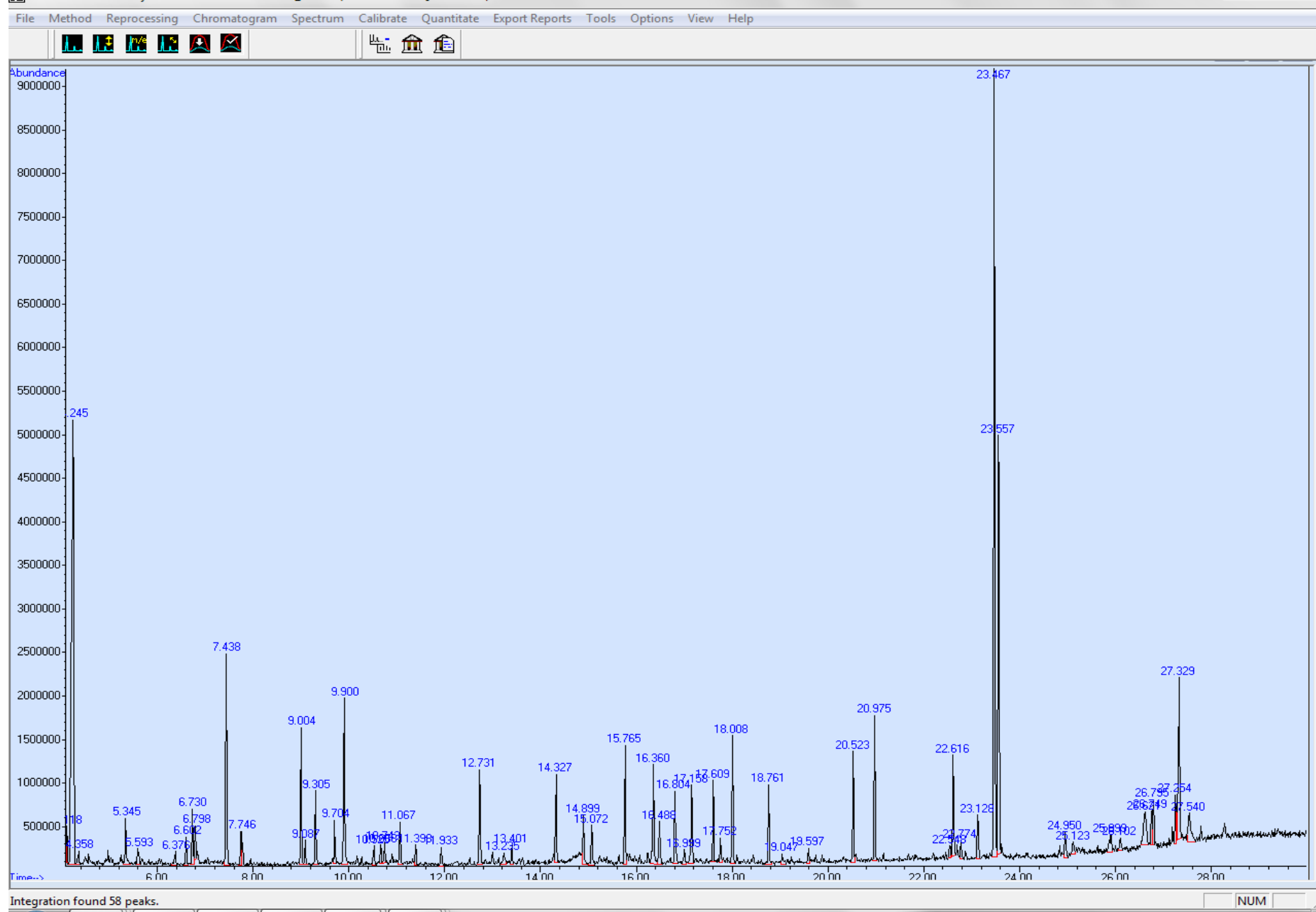


Figure 9. Total Ion Chromatogram of the sample WT25. 10x split injection. File: z113012_22.

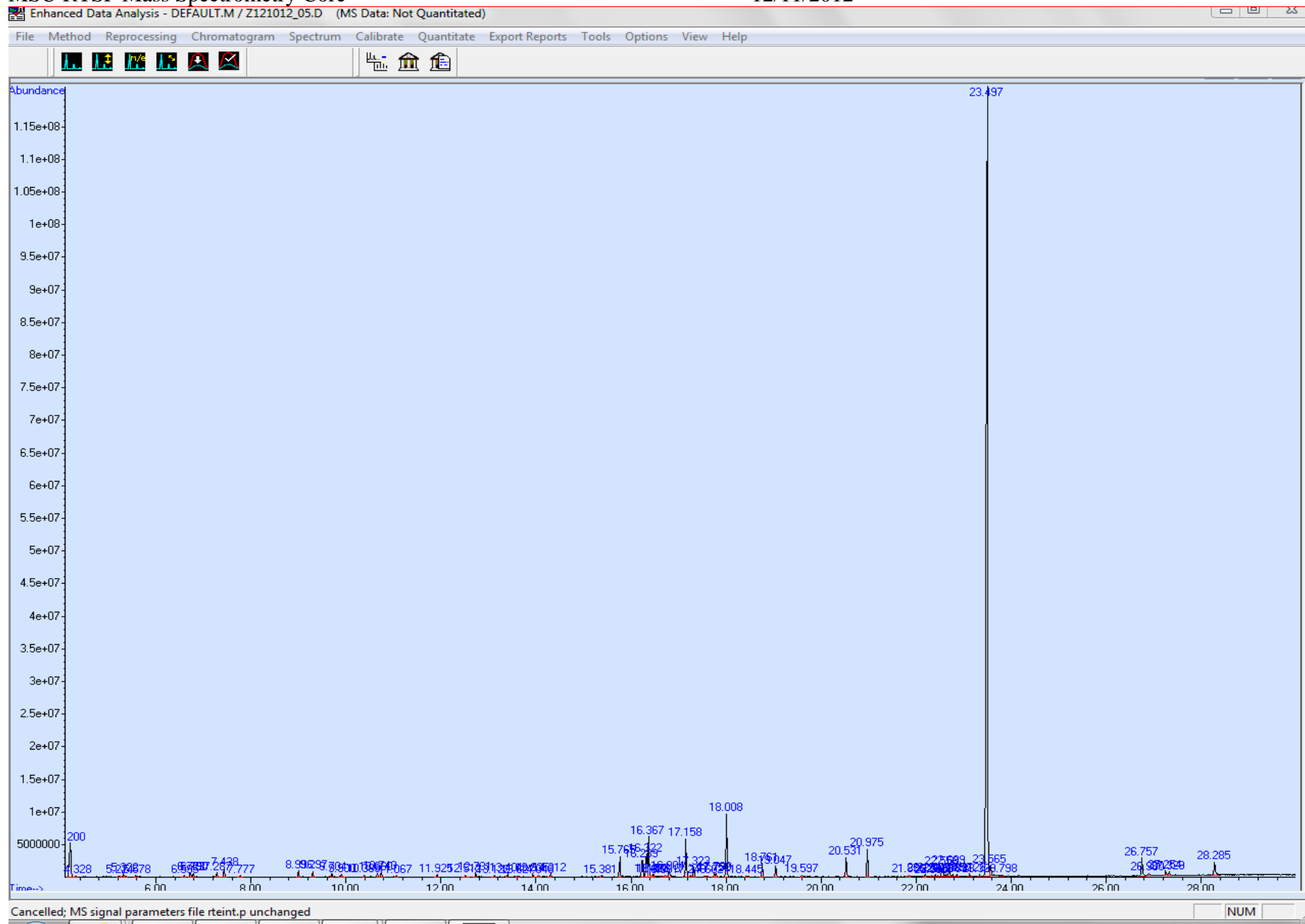


Figure 10. Total Ion Chromatogram of the sample T18-3. 10x split injection. File: z121012_05.

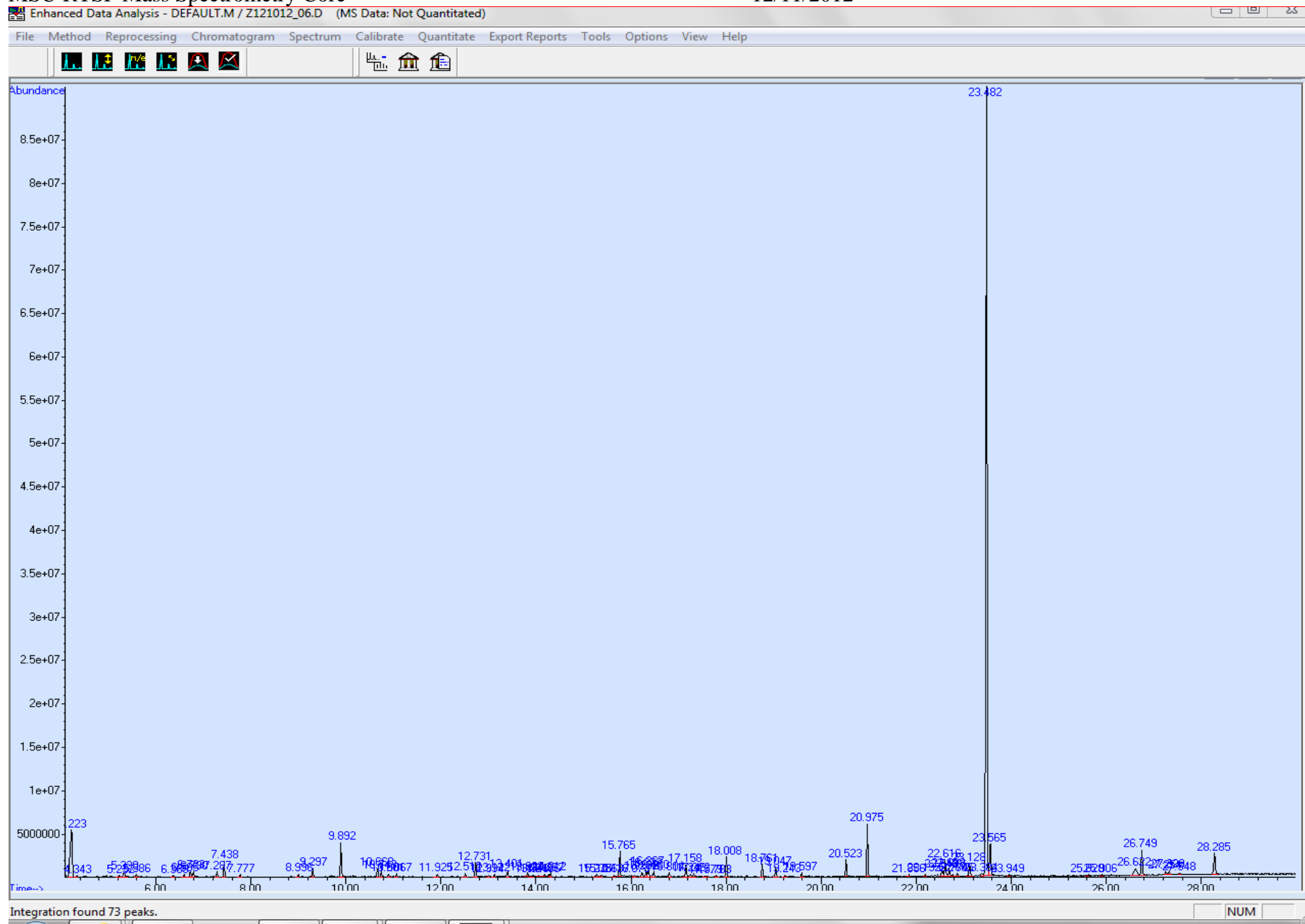


Figure 11. Total Ion Chromatogram of the sample T51-1. 10x split injection. File: z121012_06.

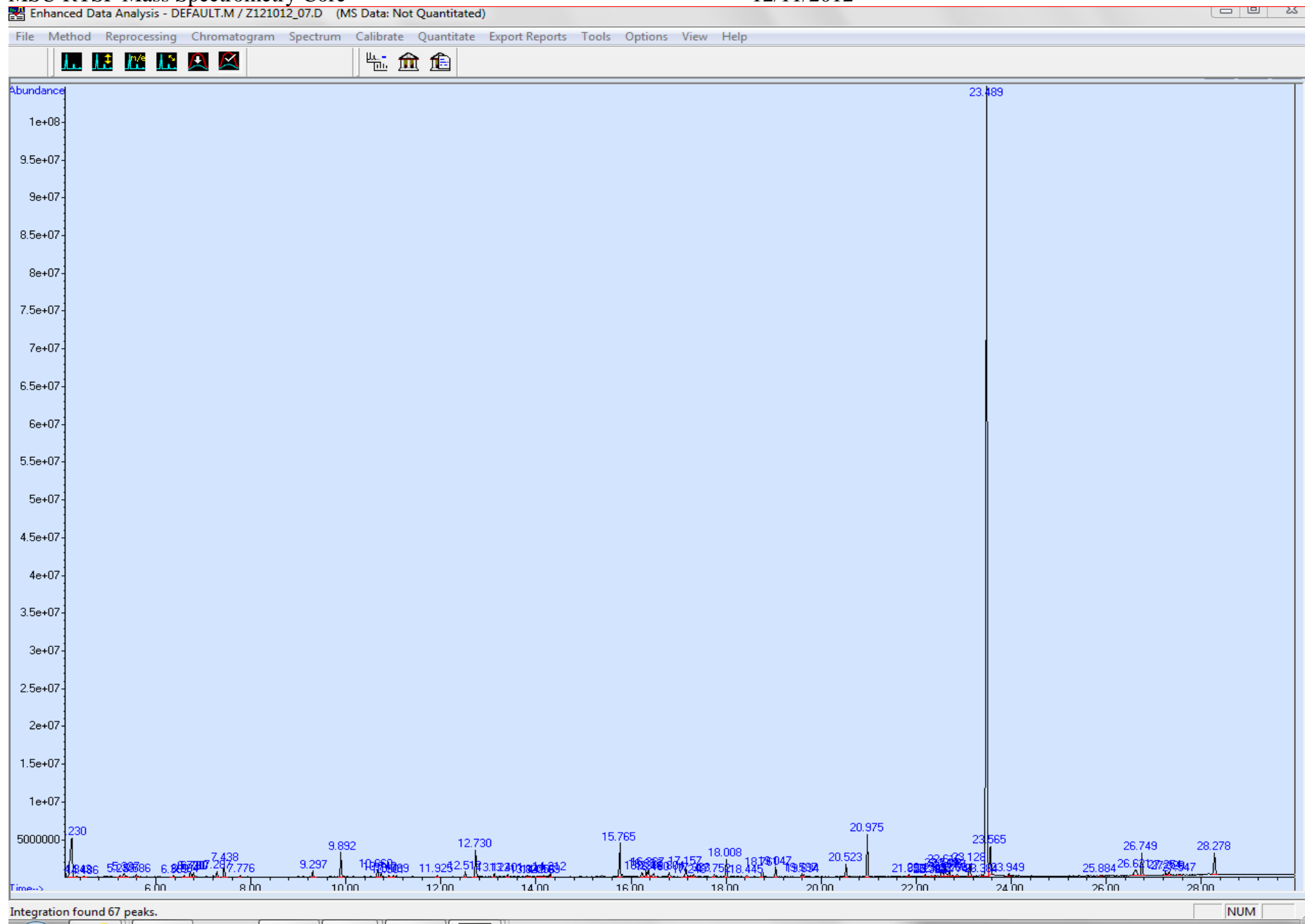


Figure 12. Total Ion Chromatogram of the sample T51-2. 10x split injection. File: z121012_07.

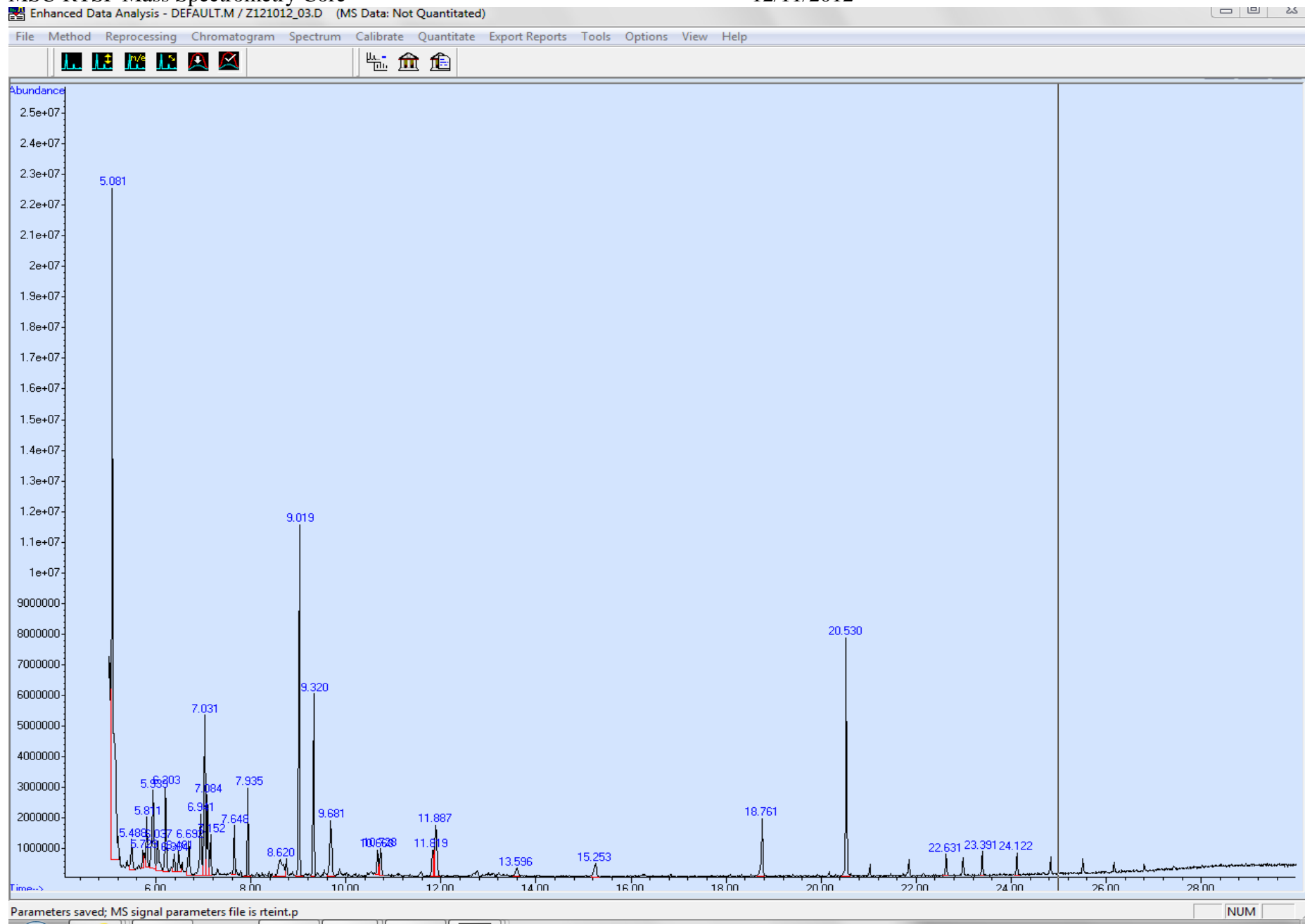


Figure 13. Total Ion Chromatogram of the MSTFA blank. Splitless injection. File: z121012_03.

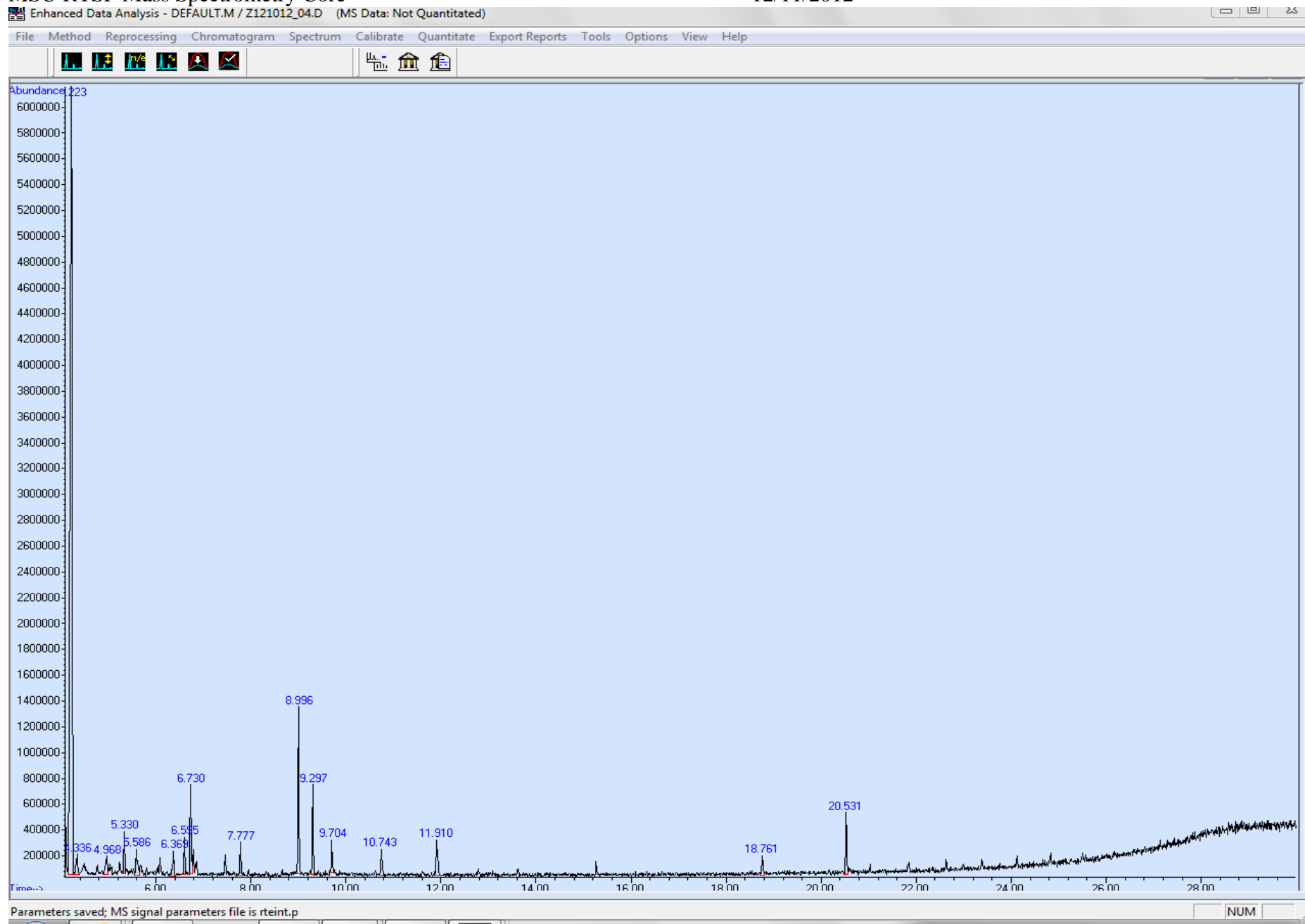


Figure 14. Total Ion Chromatogram of the MSTFA blank. 10x split injection. File: z121012_04.

Table 1. Automated database search for sample '1JT beta'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_23.D						
PBM Apex						
Mon Dec 10 15:45:37 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	5.0887	2.4861	Acetamide, 2,2,2-trifluoro-N,N-bis(trimethylsilyl)-	96933	021149-38-2	81
2	5.3747	0.3774	Silane, trimethyl(3-octyloxy)-	58248	1000157-39-9	70
3	5.4651	0.355	2-Methyl-1-butanol, 3-t-butyldimethylsilyloxy-	69561	085576-59-6	43
4	5.7888	0.8925	Butyrolactone	1620	000096-48-0	87
5	5.9394	1.4148	Silamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	83
6	6.0222	0.5233	Ethanol, 2-(trimethylsilyl)-	8511	002916-68-9	50
7	6.1201	0.6828	(Z)-Bis-1,2-(trimethylsilyloxy)ethylene	60281	026327-98-0	52
8	6.1879	1.4609	Cyclohexanecarboxylic acid, 1-methyl-2-oxo-, ethyl ester	45647	005453-94-1	15
9	6.6923	0.4703	Tetrasiloxane, decamethyl-	130465	000141-62-8	90
10	6.9408	0.935	4-Fluorobenzoic acid, 3,5-difluorophenyl ester	93138	1000299-04-8	27
11	7.0311	1.7146	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71659	017887-80-8	90
12	7.0838	3.2525	Propanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	81450	017596-96-2	76
13	7.1441	0.4703	Butanoic acid, (tetrahydro-2-furanyl)methyl ester	38339	002217-33-6	32
14	7.3022	2.294	Disiloxane, ethylpentamethyl-	40591	006231-60-3	72
15	7.513	1.73	Silamine, N-(2,2-dimethylpropyl)-1,1,1-trimethyl-	29324	074421-07-1	22
16	7.656	0.5381	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	59
17	7.9421	0.6625	Silane, bromotriethyl-	53057	001112-48-7	37
18	7.9873	0.265	Trimethylsilyl ether of glycerol	129248	006787-10-6	47
19	8.5971	0.3421	Succinic acid, 2-hydroxy-3-methyl-, diethyl ester	60356	1000196-85-6	35
20	9.0112	4.91	Propanedioic acid, bis(trimethylsilyl) ester	90960	018457-04-0	91
21	9.2597	1.0552	3,7-Dioxa-2,8-disilanonan-5-one, 2,2,8,8-tetramethyl-	81446	017877-42-8	93
22	9.3274	1.8127	Silamine, N-[2-[3,4-bis[(trimethylsilyl)oxy]phenyl]ethyl]-1,1,1-trimethyl-N-(trimethylsilyl)-	178791	055606-74-1	64
23	9.6964	1.061	3-Propyl-6-methyl-1,2,3,4-tetrahydro-.gamma.-carboline	77394	1000071-40-2	50
24	9.8695	1.4053	Trimethylsilyl ether of glycerol	129246	006787-10-6	80
25	10.118	0.2505	1H-Indole, 2,3,5-trimethyl-1-(trimethylsilyl)-	79283	074367-58-1	64

26	10.1481	0.3903	1H-Indole, 2,3,5-trimethyl-1-(trimethylsilyl)-	79283	074367-58-1	78
27	10.4718	0.6234	Butanedioic acid, bis(trimethylsilyl) ester	99521	040309-57-7	78
28	10.517	0.654	Butanedioic acid, bis(trimethylsilyl) ester	99522	040309-57-7	94
29	10.6149	0.455	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137602	038191-87-6	68
30	10.6525	0.8373	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137602	038191-87-6	91
31	10.6977	1.5342	1,4-Dimethoxy-2-(methylthio)-benzene	46480	002570-42-5	27
32	10.7353	1.8118	Propanenitrile, 3-(ethylphenylamino)-	38947	000148-87-8	22
33	11.0516	0.236	L-Serine, N,O-bis(trimethylsilyl)-, trimethylsilyl ester	137174	007364-48-9	86
34	11.3075	0.2313	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4.alpha.,4a.alpha.,6.beta.)]-	69990	004674-50-4	86
35	11.6614	1.3173	3,8-Dioxa-2,9-disiladec-5-ene, 2,2,9,9-tetramethyl-, (E)-	79474	053326-59-3	51
36	11.7141	1.7848	3,8-Dioxa-2,9-disiladec-5-ene, 2,2,9,9-tetramethyl-, (E)-	79474	053326-59-3	44
37	11.8496	0.2276	9-Borabicyclo[3.3.1]nonane, 9-[(2-pyridyl)methylamino]-	77264	1000162-55-4	35
38	11.9023	0.5818	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	188706	002582-79-8	38
39	12.2185	1.3158	Propanedioic acid, bis[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	176004	042827-95-2	45
40	12.6402	0.4472	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	86
41	12.7004	1.6417	Malic acid, tris(trimethylsilyl) ester	152350	065143-63-7	91
42	13.1973	0.2988	L-Proline, 5-oxo-1-(trimethylsilyl)-, trimethylsilyl ester	107236	030274-77-2	42
43	13.3855	1.2192	1-Allyl-2-imino-10-oxo-1,10-dihydro-2H-1,9,10a-triazaanthracene-3-carboxylic acid, methyl ester	130761	1000311-49-4	47
44	13.521	0.4658	Tris(trimethylsiloxy)ethylene	119316	069097-20-7	90
45	13.777	5.446	Ribo-hexos-3-ulose, 2,4,5,6-tetrakis-O-(trimethylsilyl)-, bis(O-methyloxime)	185858	062108-14-9	53
46	14.2664	0.7133	Myo-inositol, 5-deoxy-1,2,3,4,6-pentakis-O-(trimethylsilyl)-	185862	114656-62-1	42
47	15.072	0.334	Trimethylsilyl ether of glycerol	129245	006787-10-6	59
48	15.2527	0.2542	Carbonic acid, dithio-, S-methyl O-(2-methylcyclohexyl) ester, cis-	60364	015288-12-7	41
49	15.3581	0.4388	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, epi-	188709	029267-01-4	40
50	15.9679	0.277	Silane, trimethyl[1-methyl-2-oxo-2-(trimethylsilyl)ethoxy]-, (R)-	70223	055255-93-1	43
51	16.0131	0.3254	Butane, 1,2,3,4-tetrakis[(trimethylsilyl)oxy]-	173327	018547-29-0	50
52	16.0809	0.8015	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	145437	038165-93-4	43
53	16.2314	1.624	Pseudo uridine penta-tms	188529	053294-25-0	59
54	16.3218	1.4297	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	80
55	16.6681	0.8776	.beta.-D-Galactofuranose, 1,2,3,5,6-pentakis-O-(trimethylsilyl)-	186559	007045-52-5	78
56	16.8036	0.3662	Butane, 1,2,3,4-tetrakis[(trimethylsilyl)oxy]-	173327	018547-29-0	14
57	16.9994	0.3505	Silane, dimethylbis[(trimethylsilyl)methyl]-	79482	005695-47-6	38
58	17.1575	1.501	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	180129	019127-15-2	91

59	17.2855	1.0466	Xylonic acid, 2,3,4-tris-O-(trimethylsilyl)-, .delta.-lactone, D-	158611	032384-59-1	62
60	17.5866	0.4814	.alpha.-D-Glucopyranuronic acid, 1,2,3,4-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester	187122	052842-25-8	46
61	17.8878	0.5707	D-Xylofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178318	056271-68-2	45
62	18.0083	1.9139	Glucopyranose, pentakis-O-trimethylsilyl-	186534	1000157-49-7	94
63	18.0986	1.2151	.beta.-DL-Arabinofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164979	056271-63-7	50
64	18.2492	1.3864	3-Bromo-5-ethoxy-4-hydroxybenzaldehyde	88284	003111-37-3	86
65	18.7612	3.5275	Hexadecanoic acid, trimethylsilyl ester	141309	055520-89-3	98
66	18.8364	0.3401	Arabinose, 2,3,4,5-tetrakis-O-(trimethylsilyl)-	178314	001768-95-2	58
67	19.7474	0.2274	1-Dimethyl(octyl)silyloxyoctadecane	178714	1000280-39-7	68
68	20.3272	0.2866	1-Ethyl-2-pentamethyldisilanyloxycyclohexane	97176	1000216-94-6	43
69	20.538	6.6852	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	97
70	20.9747	0.3323	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186538	006736-97-6	80
71	21.848	0.3001	Tetracosane	146922	000646-31-1	91
72	22.616	4.1365	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	38
73	22.8719	0.4865	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	47
74	23.1279	3.3131	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	49
75	23.3914	0.7902	Hexacosane	159835	000630-01-3	93
76	23.4743	3.4593	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	90
77	23.5646	3.6202	[4-Bromo-2-(hydrazono-phenyl-methyl)-phenyl]-carbamic acid, ethyl ester	157451	1000318-37-6	86
78	24.1217	0.6702	Tricosane	139232	000638-67-5	95
79	24.8295	0.6213	Heptadecane, 9-octyl-	153748	007225-64-1	94
80	25.5071	0.3773	Nonacosane	173140	000630-03-5	96
81	26.6063	0.5227	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'- bis(1-methylethyl)-	188504	027864-29-5	38
82	27.2613	0.9198	1-(3-Methylbutyl)-2,3,4-trimethylbenzene	50022	107997-59-1	38
83	28.2702	0.3515	D-Ribose, 2,3,4,5-tetrakis-O-(trimethylsilyl)-	178312	033648-69-0	30
84	28.368	0.2438	.beta.-Sitosterol trimethylsilyl ether	183578	002625-46-9	49

Table 2. Automated database search for sample '3JT beta'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_24.D						
PBM Apex						
Mon Dec 10 15:44:32 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	5.0361	0.4382	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39867	000920-68-3	90
2	5.0738	2.2239	Acetamide, 2,2,2-trifluoro-N,N-bis(trimethylsilyl)-	96932	021149-38-2	92
3	5.4653	0.4009	(3-Methoxyphenyl)acetonitrile	21681	019924-43-7	30
4	5.7137	0.2933	1,3-Dichloro-2-propanol, trimethylsilyl ether	57395	007453-13-6	38
5	5.7664	0.5029	Butyrolactone	1626	000096-48-0	87
6	5.9321	1.5051	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	94
7	5.9998	0.4289	2-Dimethyl(prop-2-enyl)silyloxypropane	28864	098582-95-7	47
8	6.173	1.0289	Iron, (.eta.6-benzene)[(1,2,3,4-.eta.)-1,3-cyclohexadiene]-	66975	071265-76-4	25
9	6.685	0.4787	Tetrasiloxane, decamethyl-	130465	000141-62-8	90
10	6.9334	0.9153	Benzoyl chloride, 4-fluoro-	28675	000403-43-0	43
11	7.0238	1.666	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71659	017887-80-8	90
12	7.0765	1.2492	Butanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90121	055133-94-3	72
13	7.1367	0.4702	Furan, tetrahydro-2-(methoxymethyl)-	7978	019354-27-9	47
14	7.6411	0.6134	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	59
15	7.9348	0.6335	1-(2,5-Dimethoxyphenyl)-propanol	54137	089106-42-3	32
16	8.6726	0.523	2-Pyrrolidinone	1514	000616-45-5	47
17	9.0265	4.9582	Propanedioic acid, bis(trimethylsilyl) ester	90960	018457-04-0	46
18	9.1168	0.7943	L-Valine, N-(trimethylsilyl)-, trimethylsilyl ester	99068	007364-44-5	86
19	9.3276	1.7949	Cadaverine tri-TMS	135437	1000141-25-1	64
20	9.5685	0.287	Urea, N,N'-bis(trimethylsilyl)-	60203	018297-63-7	93
21	9.6062	0.4521	Urea, N,N'-bis(trimethylsilyl)-	60203	018297-63-7	64
22	9.7266	1.1289	5-Methoxy-thiophene-2-carboxamide	28085	076371-65-8	37
23	9.8772	3.6163	Trimethylsilyl ether of glycerol	129245	006787-10-6	87
24	10.1709	0.5239	L-Isoleucine, N-(trimethylsilyl)-, trimethylsilyl ester	108551	007483-92-3	80
25	10.2687	3.3272	L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester	97807	007364-47-8	93
26	10.329	0.5768	Butanoic acid, 4-[(trimethylsilyl)amino]-, trimethylsilyl ester	89623	039538-11-9	90

27	10.5172	0.4206	Butanedioic acid, bis(trimethylsilyl) ester	99521	040309-57-7	87
28	10.6527	0.2207	Urea, N,N'-bis(trimethylsilyl)-	60204	018297-63-7	62
29	10.7355	0.6697	Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-	39070	021693-51-6	25
30	11.0517	1.5178	Serine tritms	137173	064625-17-8	53
31	11.3755	0.5602	N,O,O-Tris(trimethylsilyl)-L-threonine	145071	007537-02-2	53
32	11.6541	0.2607	3-Chloro-1,2-propanediol, di(trimethylsilyl) ether	95060	073639-52-8	64
33	11.7143	1.2949	3,8-Dioxa-2,9-disiladecane, 2,2,9,9-tetramethyl-	80696	018001-91-7	43
34	11.9025	0.6288	Cyclopenta(cd)pyrene, 3,4-dihydro-	77470	025732-74-5	30
35	12.2338	0.2716	1,2,3-Propanetricarboxylic acid, 2-[(trimethylsilyl)oxy]-, tris(trimethylsilyl) ester	182939	014330-97-3	27
36	12.6403	0.5185	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	96
37	12.7006	4.2228	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	96
38	12.9641	0.2798	1-Morpholin-4-yl-3-(naphthalen-1-yloxy)propan-2-ol	116648	1000311-32-3	22
39	13.19	0.3992	L-Proline, 5-oxo-1-(trimethylsilyl)-, trimethylsilyl ester	107238	030274-77-2	68
40	13.3857	0.5619	1-Allyl-2-imino-10-oxo-1,10-dihydro-2H-1,9,10a-triazaanthracene-3-carboxylic acid, methyl ester	130761	1000311-49-4	28
41	13.5212	0.2741	2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv.	176015	038191-88-7	52
42	13.7847	6.8788	Xylulose tetrakis(trimethylsilyl)-	178306	1000141-49-4	47
43	14.3946	0.5511	N,O-Bis(trimethylsilyl)-L-phenylalanine	130125	007364-51-4	83
44	14.8614	0.5981	Stephaboline	144125	036871-86-0	74
45	16.0811	0.8898	L-Gluconic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181666	056298-43-2	70
46	16.2316	2.7825	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	78
47	16.322	2.5225	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	72
48	16.6984	1.1412	Glucufuranoside, methyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-, .alpha.-D-	183112	006736-96-5	59
49	16.8038	0.5345	D-Xylose, tetrakis(trimethylsilyl)-	178308	018623-22-8	45
50	16.9996	0.3513	Ribitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	185219	032381-53-6	50
51	17.1125	1.0538	D-Xylose, tetrakis(trimethylsilyl)-	178308	018623-22-8	64
52	17.1577	1.4366	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	93
53	17.2555	0.4401	.beta.-DL-Lyxopyranose, 1,2,3,4-tetrakis-O-(trimethylsilyl)-	178324	056271-66-0	81
54	17.5868	0.6154	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	43
55	17.888	2.4308	.beta.-D-Galactofuranose, 1,2,3,5,6-pentakis-O-(trimethylsilyl)-	186559	007045-52-5	72
56	18.0085	3.181	Glucopyranose, pentakis-O-trimethylsilyl-	186534	1000157-49-7	93
57	18.1063	3.7852	Silane, (1,2,4,5-cyclohexanetetrayltetraoxy)tetrakis[trimethyl-	178056	100258-68-2	50
58	18.2494	2.7488	Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178320	055399-49-0	50
59	18.7613	2.3827	Hexadecanoic acid, trimethylsilyl ester	141306	055520-89-3	95
60	18.8366	0.6128	Myo-inositol, 5-deoxy-1,2,3,4,6-pentakis-O-(trimethylsilyl)-	185862	114656-62-1	56

61	19.0474	0.7714	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	188704	002582-79-8	80
62	19.597	0.2754	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170036	010586-03-5	96
63	19.7476	0.2198	Silane, trimethyl(octadecyloxy)-	148891	018748-98-6	78
64	20.2972	0.6432	L-Tryptophan, N,1-bis(trimethylsilyl)-, trimethylsilyl ester	175473	055429-28-2	72
65	20.5382	3.7593	Octadecanoic acid, trimethylsilyl ester	155418	018748-91-9	95
66	20.5833	0.595	D-Glucitol, 1,1-di-C-octyl-2,3,4,6-tetra-O-trimethylsilyl-	189915	1000161-79-1	43
67	20.9748	2.2869	2-O-Glycerol-.alpha.-d-galactopyranoside, hexa-TMS	189811	1000098-09-0	72
68	21.1555	0.3502	D-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186546	006736-94-3	72
69	22.6161	0.4843	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	58
70	23.1281	0.6086	[4-Bromo-2-(hydrazono-phenyl-methyl)-phenyl]-carbamic acid, ethyl ester	157451	1000318-37-6	70
71	23.4669	1.1632	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	91
72	23.5573	0.8825	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	43
73	23.625	0.7632	Ethyl 2-ethoxyquinoline-4-carboxylate	88533	005471-39-6	25
74	26.6441	3.9256	1-Naphthalenecarboxaldehyde, 2,3,8-trimethoxy-6-methyl-4-(1-methylethyl)-7-[2,3,4-trimethoxy-7-methyl-5-(1-methylethyl)-2H-naphtho[1,8-bc]furan-8-yl]-	188505	040112-24-1	50
75	26.7571	2.5729	.alpha.-D-Glucopyranoside, methyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	183103	002641-79-4	86
76	26.8248	0.5675	Pyridine, 2,4,6-triphenyl-	129171	000580-35-8	49
77	27.2615	0.5628	Cyclobarbitol	82145	000052-31-3	22
78	27.3744	0.2699	2-Nitro-6-methyl-8-methoxy-anthra(2,1-b)furan	129030	1000148-74-3	53
79	27.5551	1.0683	5-p-Methoxyanilido-7-amino-8-5H-quinolone	111213	1000254-45-9	11
80	28.2779	0.3606	.alpha.-D-Glucopyranuronic acid, 1,2,3,4-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester	187124	052842-25-8	38

Table 3. Automated database search for sample '6JT beta'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_25.D						
PBM Apex						
Mon Dec 10 15:50:01 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	5.0662	0.2524	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	62
2	5.1038	1.5754	Acetamide, 2,2,2-trifluoro-N,N-bis(trimethylsilyl)-	96932	021149-38-2	95
3	5.3749	0.2462	Silane, ethoxytriethyl-	29960	000597-67-1	59
4	5.4652	0.1668	Silane, (1,1-dimethylethyl)dimethyl(1-phenylpropoxy)-	92055	136116-42-2	43
5	5.7363	0.1759	Benzamide, 4-fluoro-N-(5H-tetrazol-5-yl)-	62321	1000262-68-4	41
6	5.7889	0.3976	Butyrolactone	1620	000096-48-0	87
7	5.9471	0.6926	3H,6H-Thieno[3,4-c]isoxazole, 3a,4-dihydro-6-(1-methylethyl)-	37406	127865-49-0	72
8	6.0224	0.2491	Ethanol, 2-(trimethylsilyl)-	8511	002916-68-9	50
9	6.1277	0.3615	(Z)-Bis-1,2-(trimethylsilyloxy)ethylene	60281	026327-98-0	87
10	6.188	0.961	N-(2-Chloroethyl)-N-ethylaniline	45198	000092-49-9	32
11	6.7	0.3313	Methyltris(trimethylsiloxy)silane	130466	017928-28-8	58
12	6.9484	0.6641	4-Fluorobenzoic acid, 3,4-dichlorophenyl ester	114317	1000307-45-0	38
13	7.0312	1.22	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71656	017887-80-8	91
14	7.0839	1.4488	Butane, 2,3-bis(trimethylsiloxy)-	80688	053274-85-4	72
15	7.1517	0.3072	2-Butanol, 3-(2,2-dimethylpropoxy)-	30037	074793-66-1	40
16	7.3098	5.306	Acetic acid, [(trimethylsilyl)oxy]-, trimethylsilyl ester	71601	033581-77-0	91
17	7.5131	0.8521	Butanoic acid, 4-[(trimethylsilyl)amino]-, trimethylsilyl ester	89624	039538-11-9	27
18	7.6561	0.3892	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	59
19	7.9422	0.43	Cyclohexene, 3-methyl-1-(trimethylsilyloxy)-	45692	055373-58-5	14
20	7.9949	0.1422	Trisilane, octamethyl-	60283	003704-44-7	45
21	8.3864	0.2231	Butanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90127	055133-94-3	90
22	8.6048	0.1954	Quinoline, 4-methyl-, 1-oxide	29141	004053-40-1	35
23	9.0113	5.9186	Propanedioic acid, bis(trimethylsilyl) ester	90962	018457-04-0	86
24	9.1167	0.1609	L-Valine, N-(trimethylsilyl)-, trimethylsilyl ester	99068	007364-44-5	50
25	9.2598	0.6229	3,7-Dioxa-2,8-disilanonan-5-one, 2,2,8,8-tetramethyl-	81444	017877-42-8	90
26	9.3351	1.2563	.delta. Amino levulinic acid tri-TMS	151059	1000141-47-1	64

27	9.5685	0.2347	Urea, N,N'-bis(trimethylsilyl)-	60204	018297-63-7	59
28	9.6965	0.6521	Quinoline, 2,7-dimethyl-	27987	000093-37-8	40
29	9.8772	1.5335	Trimethylsilyl ether of glycerol	129246	006787-10-6	83
30	10.1482	0.5731	Benzene, 1,2,4,5-tetrakis(1-methylethyl)-	89465	000635-11-0	47
31	10.2611	0.2384	L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester	97807	007364-47-8	81
32	10.4795	0.5009	Butanedioic acid, bis(trimethylsilyl) ester	99522	040309-57-7	96
33	10.5171	0.6589	Butanedioic acid, bis(trimethylsilyl) ester	99522	040309-57-7	96
34	10.6526	1.301	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137600	038191-87-6	91
35	10.7053	0.7356	1-(2-Acetyl-3-methylphenyl)-1H-pyridin-2-one	76563	1000306-70-8	25
36	10.7355	1.1744	[1,1'-Biphenyl]-2-methanol	46061	002928-43-0	27
37	10.9839	0.2766	2-Butenedioic acid (E)-, bis(trimethylsilyl) ester	98247	017962-03-7	64
38	11.0441	0.3419	Serine tritms	137173	064625-17-8	74
39	11.2625	0.2701	Butanoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90125	055133-95-4	47
40	11.3077	0.1888	2(3H)-Furanone, dihydro-3,4-bis[(trimethylsilyl)oxy]-, trans-	99529	055220-79-6	87
41	11.669	1.3428	3-Chloro-1,2-propanediol, di(trimethylsilyl) ether	95060	073639-52-8	58
42	11.7142	2.5003	3,8-Dioxa-2,9-disiladecane, 2,2,9,9-tetramethyl-	80696	018001-91-7	43
43	11.9024	0.4897	3,8-Dioxa-2,9-disiladecane, 2,2,9,9-tetramethyl-	80696	018001-91-7	38
44	12.2187	1.1173	2-Hydroxycyclohexane-1-carboxylic acid, bis(trimethylsilyl) deriv.	116912	058877-75-1	47
45	12.452	0.2378	Gluconic acid, 2-methoxime, tetra(trimethylsilyl)-, trimethylsilyl ester	188023	1000062-87-7	50
46	12.6478	0.3822	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	90
47	12.7005	1.679	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	97
48	12.8812	0.181	Butane, 1,2,3,4-tetrakis[(trimethylsilyl)oxy]-	173326	018547-29-0	53
49	12.9941	0.2126	1,4-Diboracyclohexane, 1,4-diethyl-2,5-bis(trimethylsilyl)-	111648	1000160-14-7	59
50	13.22	0.3849	L-Proline, 5-oxo-1-(trimethylsilyl)-, trimethylsilyl ester	107238	030274-77-2	47
51	13.3932	0.5289	Lycopodan-5-one, 12-hydroxy-15-methyl-, (12.alpha.,15R)-	100653	021061-90-5	92
52	13.5212	0.7568	2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv.	176017	038191-88-7	91
53	13.7846	6.815	Trimethylsilyl ether of glycerol	129247	006787-10-6	38
54	14.2665	0.5855	Per-O-(trimethylsilyl)-.beta.-l-idofuranuronic acid	187103	1000072-41-3	38
55	14.4095	0.1555	Propanoic acid, 3-[(tert-butyldimethylsilyl)amino]-2-methyl-, tert-butyldimethylsilyl ester, (.+-.)-	142883	1000143-22-2	43
56	15.0646	0.3258	Xylulose tetrakis(trimethylsilyl)-	178306	1000141-49-4	72
57	15.3657	0.3753	D-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186546	006736-94-3	59
58	15.5314	0.1591	O,O,O'-Tris-trimethylsilylmalonate	136517	040333-06-0	64
59	15.8175	0.395	Mannonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181662	055515-30-5	80
60	15.9756	0.2452	.beta.-D-Galactofuranoside, ethyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-	184216	055493-81-7	47

61	16.081	2.0552	Gulonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181659	055528-75-1	60
62	16.2315	0.9826	.beta.-DL-Arabinofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164979	056271-63-7	64
63	16.3219	0.9175	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	78
64	16.6607	0.4355	.alpha.-DL-Lyxofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164977	056390-03-5	80
65	16.8113	0.2236	1,11-Undecanedioic acid, di(trimethylsilyl) ester	156954	106450-25-3	40
66	16.9995	0.4878	Gulonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181659	055528-75-1	46
67	17.1576	0.8905	.alpha.-D-Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186560	032166-80-6	91
68	17.2856	0.8659	.alpha.-L-Galactofuranose, 6-deoxy-1,2,3,5-tetrakis-O-(trimethylsilyl)-	180139	056227-36-2	64
69	17.5867	0.6334	Xylonic acid, 2,3,4-tris-O-(trimethylsilyl)-, .delta.-lactone, D-	158611	032384-59-1	30
70	17.6771	0.2237	Altronic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181661	055528-73-9	50
71	17.79	0.1714	Cinnamic acid, p-(trimethylsiloxy)-, trimethylsilyl ester	129432	010517-30-3	95
72	17.8879	1.0107	Mannonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181662	055515-30-5	56
73	18.0084	1.1134	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	91
74	18.1062	1.3852	Per-O-(trimethylsilyl)-.alpha.-l-idofuranuronic acid	187104	1000072-40-9	53
75	18.2493	1.8066	.beta.-DL-Arabinofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164979	056271-63-7	64
76	18.7613	1.5869	Hexadecanoic acid, trimethylsilyl ester	141309	055520-89-3	98
77	18.8365	0.4466	D-Glycero-L-manno-Heptonic acid, 2,3,5,6,7-pentakis-O-(trimethylsilyl)-, .gamma.-lactone	187577	027531-31-3	59
78	19.0474	0.2212	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	188704	002582-79-8	87
79	19.2356	0.1682	2-Deoxy-galactopyranose, tetrakis(trimethylsilyl)	180128	1000079-29-5	38
80	19.597	0.2435	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170036	010586-03-5	94
81	20.3273	0.2277	.alpha.-Linolenic acid, trimethylsilyl ester	152701	097844-13-8	95
82	20.5381	2.6554	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	96
83	20.5757	0.1491	.alpha.-DL-Lyxofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164977	056390-03-5	45
84	20.9748	0.2704	2-O-Glycerol-.alpha.-d-galactopyranoside, hexa-TMS	189811	1000098-09-0	93
85	21.1555	0.2992	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186540	006736-97-6	72
86	22.6236	5.8505	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	58
87	22.8721	0.8975	3-Bromo-5-ethoxy-4-hydroxybenzaldehyde	88284	003111-37-3	53
88	23.0753	0.2329	Benzimidazole, 2,3-dihydro-1,3-dimethyl-2-(1-phenylpyrazol-4-yl)-	118561	1000260-34-1	32
89	23.1356	5.2002	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	52
90	23.2635	0.6096	Thymol-.beta.-d-glucopyranoside, tetrakis(O-trimethylsilyl)-	188461	1000108-99-1	12
91	23.384	0.5397	Xylonic acid, 2,3,4-tris-O-(trimethylsilyl)-, .delta.-lactone, D-	158611	032384-59-1	20
92	23.4744	3.5691	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl	190724	019159-25-2	90

			2,3,4,6-tetrakis-O-(trimethylsilyl)-			
93	23.5722	5.9025	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	58
94	24.1218	0.2483	Eicosane, 1,20-dibromo-	178366	014296-16-3	37
95	24.6639	0.2143	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	38
96	24.8371	0.1497	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	59
97	24.935	0.1394	D-Glucose, 4-O-[2,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-galactopyranosyl]-2,3,5,6-tetrakis-O-(trimethylsilyl)-	190717	055669-93-7	68
98	25.4394	0.1855	Xylopyranoside, methyl 2,3,4-tris-O-(trimethylsilyl)-, .alpha.-D-	164978	018082-35-4	64
99	25.5373	0.257	.alpha.-D-Galactopyranosiduronic acid, methyl 2,3,4-tris-O-(trimethylsilyl)-, methyl ester	178304	056271-13-7	80
100	26.629	1.9233	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-	188504	027864-29-5	64
101	26.7494	0.2785	D-Glucopyranose, 4-O-[2,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-galactopyranosyl]-1,2,3,6-tetrakis-O-(trimethylsilyl)-	190721	055529-68-5	72
102	26.8247	0.1451	Cobalt, acetylacetonato-(ethyltetramethylcyclopentadienyl)-	128954	1000164-04-5	55
103	27.0807	0.1528	.alpha.-Tocopherol (vitamin E), trimethylsilyl derivative	184680	002733-26-8	96
104	27.2614	0.4212	Stannane, tetrapropyl-	119351	002176-98-9	43
105	27.555	0.5166	5-(4-tert-Butyl-benzylsulfanyl)-[1,3,4]thiadiazol-2-ylamine	111078	1000294-26-6	14
106	27.6153	0.225	Maltose, octakis(trimethylsilyl)-	190711	033428-94-3	35
107	28.2778	0.5861	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	68
108	28.3682	0.188	.beta.-Sitosterol trimethylsilyl ether	183580	002625-46-9	35

Table 4. Automated database search for sample '2JT CHO'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_17.D						
PBM Apex						
Mon Dec 10 21:46:23 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2379	16.0742	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	94
2	5.3371	0.7554	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	46
3	6.3685	0.3643	Trimethyl[4-(2-methyl-4-oxo-2-pentyl)phenoxy]silane	101262	1000283-54-9	53
4	6.6019	0.4469	Carbamothioic chloride, dimethyl-	9762	016420-13-6	38
5	6.7299	1.0506	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71657	017887-80-8	80
6	6.7977	0.7104	Butane, 2,3-bis(trimethylsiloxy)-	80690	053274-85-4	64
7	7.4527	0.4189	1,2-Bis(trimethylsiloxy)ethane	61756	007381-30-8	40
8	7.7764	0.4359	Silane, (2-bromoethoxy)trimethyl-	54622	034714-03-9	16
9	8.6046	0.3585	1-Dimethyl(butyl)silyloxybutane	48407	1000280-35-2	37
10	8.9735	8.0706	Propanedioic acid, bis(trimethylsilyl) ester	90960	018457-04-0	91
11	9.0865	0.3716	2,3,1-Benzodiazaborine, 1,2-dihydro-1-methyl-	20291	004885-27-2	64
12	9.2521	0.5455	Butane, 1,2,4-tris(trimethylsiloxy)-	137637	033581-75-8	40
13	9.3048	1.0986	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118833	005630-82-0	90
14	9.5909	0.4129	1H-1-Silaindene, 2,3-dihydro-1-methyl-1-propyl-	49910	061141-64-8	38
15	9.877	2.7907	Trimethylsilyl ether of glycerol	129245	006787-10-6	70
16	10.1556	0.5678	12-(5-Ethyl-2-tetrahydrofuranyl)-7,12-bis(trimethylsilyloxy)-9(Z)-dodecenoic acid,methyl ester	183510	1000281-45-7	56
17	10.2685	0.5372	L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester	97807	007364-47-8	40
18	10.5245	0.4374	Butanedioic acid, bis(trimethylsilyl) ester	99520	040309-57-7	86
19	10.6676	0.6069	Propanoic acid, 3-(trimethylsilyl)-, ethyl ester	39406	017728-88-0	27
20	10.7428	0.4571	3-Chlorobicyclo(2.2.1)heptan-2-one oxime	29242	010499-35-1	25
21	11.7291	1.8529	3,8-Dioxa-2,9-disiladec-5-ene, 2,2,9,9-tetramethyl-, (E)-	79474	053326-59-3	55
22	11.9324	0.406	Naphthacene	77459	000092-24-0	43
23	12.2562	0.3672	3-Ethyl-3-hydroxyglutaric acid tri(trimethylsilyl) deriv.	168884	087764-49-6	38
24	12.7305	4.7573	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	152353	038166-11-9	83
25	13.2198	0.9982	Butanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90126	055133-94-3	25

26	13.8146	9.2016	Butanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90126	055133-94-3	37
27	16.0808	0.8638	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	48
28	16.2389	4.0214	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	83
29	16.3218	3.1841	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	56
30	16.3669	6.6244	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	186553	030645-02-4	80
31	16.7057	1.6895	Per-O-(trimethylsilyl)-.alpha.-D-mannopyranuronic acid	187105	068398-75-4	43
32	16.9692	0.514	Glucofuranoside, methyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-, .alpha.-D-	183112	006736-96-5	40
33	17.1123	0.7678	Ribitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	185223	032381-53-6	62
34	17.1575	4.0578	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	94
35	17.2478	0.9739	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	83
36	17.3382	0.5077	Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, .beta.-d-	186564	001769-00-2	53
37	17.8878	1.8696	Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178320	055399-49-0	53
38	18.0082	6.9487	Glucopyranose, pentakis-O-trimethylsilyl-	186534	1000157-49-7	95
39	18.0986	2.9138	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, scyllo-	188712	014251-18-4	53
40	18.2492	1.315	D-Xylofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178318	056271-68-2	72
41	18.7611	1.5499	Hexadecanoic acid, trimethylsilyl ester	141308	055520-89-3	93
42	19.0472	0.5616	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, muco-	188711	029412-26-8	72
43	20.5304	2.2047	Octadecanoic acid, trimethylsilyl ester	155420	018748-91-9	96
44	20.9746	0.8722	2-O-Glycerol-.alpha.-d-galactopyranoside, hexa-TMS	189811	1000098-09-0	87
45	22.6159	0.6218	1-Deoxyglucose, tetrakis(trimethylsilyl)	180127	082682-67-5	47
46	23.4667	0.8831	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	83
47	23.5571	0.8662	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	27
48	26.6138	1.0982	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl- 5,5'-bis(1-methylethyl)-	188504	027864-29-5	8
49	26.7493	0.6115	1,4,6-Trimethyl-1,2,3,4-tetrahydroquinoxaline-2,3-dione	59428	004951-03-5	46
50	27.2537	0.385	1,2,3-Propatriol, 1-indol-4-yl(ether)	61982	061212-32-6	72

Table 5. Automated database search for sample '4JT CHO'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_18.D						
PBM Apex						
Mon Dec 10 22:08:44 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2381	22.8438	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39868	000920-68-3	94
2	4.351	0.5277	Silane, (2,2-dimethylpropoxy)trimethyl-	29981	018246-63-4	49
3	5.3373	1.0181	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	87
4	5.5857	0.632	Acetic acid, 2-phenoxy-, (1,7,7-trimethylbicyclo[2.2.1]hept-2-ylidenamino) ester	125493	328023-79-6	38
5	6.3687	0.4916	Tetrasiloxane, decamethyl-	130465	000141-62-8	64
6	6.6021	0.7373	4-Fluorobenzoic acid, 4-cyanophenyl ester	85963	1000307-44-9	43
7	6.7301	1.5771	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71658	017887-80-8	72
8	6.7904	0.9178	Propanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	81450	017596-96-2	78
9	7.4529	0.4808	Benzimidazole, 2-amino-1-methyl-	21622	001622-57-7	50
10	7.7767	0.6214	Silane, bromotriethyl-	53057	001112-48-7	32
11	8.9737	7.9882	Butanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	90127	055133-94-3	74
12	9.305	1.6144	Propanoic acid, 3-[bis(trimethylsilyl)amino]-2-methyl-, trimethylsilyl ester	136129	055125-15-0	86
13	9.5911	0.8484	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	72
14	9.7041	1.0298	2-Fluoro-4-nitrophenol	28076	000403-19-0	43
15	9.8772	1.6367	Trimethylsilyl ether of glycerol	129245	006787-10-6	87
16	10.2687	0.6533	L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester	97807	007364-47-8	83
17	10.743	0.5091	9-Thiabicyclo[3.3.1]nonane-2,6-dione	36719	037918-35-7	38
18	11.7293	1.5941	2-Methyl-1,4-bis(trimethylsiloxy)butane	90203	105747-05-5	46
19	11.9251	0.6289	4-(1-Adamantyl)phenyl acetate	105685	063013-56-9	17
20	12.7307	5.8029	Malic acid, tris(trimethylsilyl) ester	152350	065143-63-7	70
21	13.2351	0.5704	tert-Butylpentamethyldisiloxane	60386	067875-54-1	27
22	13.4007	0.515	Phosphenimidous amide, tris(trimethylsilyl)-	110956	050732-21-3	56
23	13.8148	7.4283	Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis[trimethyl-	91530	062185-57-3	46
24	16.081	0.8147	2-Pentenedioic acid, 2-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	157728	055590-97-1	38
25	16.2391	2.2281	D-Glycero-L-manno-Heptonic acid, 2,3,5,6,7-pentakis-O-(trimethylsilyl)-, .gamma.-lactone	187577	027531-31-3	56

26	16.322	1.9403	1H-Indole-3-carboxaldehyde, 1-(trimethylsilyl)-	69080	074367-39-8	50
27	16.3671	4.3174	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	186553	030645-02-4	78
28	16.4575	0.6573	1-Phenanthrenecarboxylic acid, 8-chloro-1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]-	151799	084114-10-3	43
29	16.7059	1.0845	Glucofuranoside, methyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-, .alpha.-D-	183112	006736-96-5	43
30	17.1577	2.1451	Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-	186545	006736-99-8	90
31	17.248	0.6666	.alpha.-D-Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186560	032166-80-6	58
32	17.888	1.7134	Silane, (1,2,4,5-cyclohexanetetrayltetraoxy)tetrakis(trimethyl-	178056	100258-68-2	64
33	18.0084	3.6739	l-Fucose, tetra-TMS-ether	180126	117307-13-8	90
34	18.0988	2.3387	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, muco-	188711	029412-26-8	52
35	18.2494	1.0362	Per-O-(trimethylsilyl)-.alpha.-l-idofuranuronic acid	187104	1000072-40-9	64
36	18.7613	2.7284	Hexadecanoic acid, trimethylsilyl ester	141311	055520-89-3	68
37	20.5306	4.554	Octadecanoic acid, trimethylsilyl ester	155420	018748-91-9	97
38	20.9748	0.7229	.beta.-D-Galactopyranoside, methyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	183109	002296-39-1	72
39	22.6161	0.7127	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	50
40	23.4669	1.125	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	43
41	23.5648	1.1881	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	27
42	26.614	2.526	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-	188504	027864-29-5	46
43	26.757	0.6998	D-Glucose, 4-O-[2,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-galactopyranosyl]-2,3,5,6-tetrakis-O-(trimethylsilyl)-	190717	055669-93-7	41
44	27.2539	1.3225	Tetrasiloxane, decamethyl-	130465	000141-62-8	50
45	27.5476	1.1372	1-Benzazirene-1-carboxylic acid, 2,2,5a-trimethyl-1a-[3-oxo-1-butenyl] perhydro-, methyl ester	101889	1000197-90-8	53

Table 6. Automated database search for sample '5JT CHO'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_19.D						
PBM Apex						
Mon Dec 10 16:37:39 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2228	27.2352	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39868	000920-68-3	94
2	5.3296	0.9775	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	56
3	5.578	0.7627	Acetamide, 2,2,2-trifluoro-N-methyl-N-(trimethylsilyl)-	56618	024589-78-4	40
4	6.5944	0.7212	2-Fluorobenzoic acid, 2-methylpropyl ester	54125	159139-43-2	43
5	6.7299	1.8348	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71659	017887-80-8	52
6	6.7902	1.0779	3,6-Dioxa-2,7-disilaoctane, 2,2,4,7,7-pentamethyl-	71663	017887-27-3	64
7	7.0612	0.8473	2-Ethyl-3-hydroxypropionic acid, di-TMS	99594	1000072-00-1	64
8	7.4527	0.7716	1-(3-Methylbutyl)-2,3,4,6-tetramethylbenzene	59883	116761-72-9	59
9	7.7764	0.7197	Indol-2-one, 5-chloro-1,3-dihydro-	34344	017630-75-0	25
10	8.9735	9.3081	Propanedioic acid, bis(trimethylsilyl) ester	90960	018457-04-0	83
11	9.3048	1.9235	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118833	005630-82-0	86
12	9.877	1.3644	Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis[trimethyl-	91530	062185-57-3	47
13	10.5245	0.8889	Butanedioic acid, bis(trimethylsilyl) ester	99522	040309-57-7	74
14	10.6676	1.1641	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137600	038191-87-6	53
15	10.7429	0.8017	Ethanone, 1-(1,4,4a,5,8,8a-hexahydro-3-phenyl-1,4:5,8-diepoxy-naphthalen-2-yl)-, (1.alpha.,4.alpha.,4a.beta.,5.beta.,8.beta.,8a.beta.)-	111949	071127-09-8	47
16	11.7291	2.5781	3,8-Dioxa-2,9-disiladec-5-ene, 2,2,9,9-tetramethyl-, (E)-	79474	053326-59-3	52
17	11.9324	0.6922	1H-Indole-3-acetonitrile, 1-(trimethylsilyl)-	77072	074367-49-0	38
18	12.7305	2.7108	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	152352	038166-11-9	91
19	13.2198	1.4635	6-Trimethylsiloxyhexanoic acid, trimethylsilyl ester	109096	150367-75-2	43
20	13.8071	10.0411	Xylulose tetrakis(trimethylsilyl)-	178306	1000141-49-4	43
21	16.0808	0.7365	Glucaric acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone, 6-(trimethylsilyl) ester	182942	056272-60-7	47
22	16.2389	1.201	Pyrimidin-2-amine, 4-methyl-6-(2-pyridylthio)-	69357	283171-79-9	49
23	16.3218	0.7581	.beta.-D-Galactofuranoside, ethyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-	184216	055493-81-7	50
24	16.3669	1.6678	.alpha.-D-Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186560	032166-80-6	64
25	16.4498	0.968	1,2,3-Propanetricarboxylic acid, 2-[(trimethylsilyl)oxy]-, tris(trimethylsilyl) ester	182940	014330-97-3	52

26	16.7057	0.8515	.beta.-D-Galactofuranoside, ethyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-	184216	055493-81-7	47
27	17.1575	1.3739	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186554	002775-90-8	81
28	17.8878	1.1452	3-Bromo-5-ethoxy-4-hydroxybenzaldehyde	88284	003111-37-3	90
29	18.0082	1.9131	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186555	002775-90-8	91
30	18.0986	1.989	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, epi-	188709	029267-01-4	37
31	18.2492	0.7217	Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178320	055399-49-0	72
32	18.7611	2.4394	Hexadecanoic acid, trimethylsilyl ester	141309	055520-89-3	83
33	20.5304	3.4113	Octadecanoic acid, trimethylsilyl ester	155418	018748-91-9	93
34	22.6084	1.4795	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	35
35	23.4667	2.3968	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	64
36	23.5571	1.4697	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	38
37	26.6213	3.4572	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl- 5,5'-bis(1-methylethyl)-	188504	027864-29-5	59
38	27.2538	0.9452	Methyl 3-bromo-1-adamantaneacetate	115660	014575-01-0	53
39	27.5474	3.1906	Pyrazolo[5,1-c][1,2,4]triazine-3,8-dicarboxylic acid, 4-amino-, diethyl ester	110987	1000302-77-3	43

Table 7. Automated database search for sample 'WT8'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_20.D						
PBM Apex						
Mon Dec 10 16:37:59 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.1099	0.4545	Trisiloxane, octamethyl-	82775	000107-51-7	86
2	4.2454	16.9158	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	94
3	4.3508	0.3464	1,13-Bis(trimethylsilyloxy)tridecane	157064	1000196-23-0	59
4	5.3371	0.7472	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	72
5	5.5931	0.3747	Iron, (.eta.6-benzene)[(1,2,3,4-.eta.)-1,3-cyclohexadiene]-	66975	071265-76-4	32
6	6.602	0.4943	2-Fluorobenzoic acid, 2-methylpropyl ester	54125	159139-43-2	38
7	6.73	1.1272	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71656	017887-80-8	91
8	6.7902	1.3218	Silane, [(1-methyl-1,3-propanediyl)bis(oxy)]bis[trimethyl-	80701	056771-47-2	86
9	6.8429	0.3442	2-Furanmethanamine, tetrahydro-	4033	004795-29-3	40
10	7.4377	1.7542	Bis(trimethylsilyl)sarcosine	80604	007364-43-4	86
11	7.7765	0.4658	Acetamide, N,N-diphenyl-	65088	000519-87-9	22
12	9.0037	2.0929	1-Phenyl-3,9-dihydro-purine-2,6-dione	76905	1000317-91-3	38
13	9.2522	0.3882	3,7-Dioxa-2,8-disilanonan-5-one, 2,2,8,8-tetramethyl-	81446	017877-42-8	87
14	9.3049	1.2158	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118832	005630-82-0	80
15	9.9072	2.7451	Silanol, trimethyl-, phosphate (3:1)	133671	010497-05-9	95
16	10.1556	0.3645	Pentitol, 3-desoxy-tetrakis-O-(trimethylsilyl)-	176035	1000151-31-7	59
17	10.7429	0.4313	Oxazole, 5-methyl-2-phenyl-	29120	005221-67-0	22
18	11.0666	0.452	L-Serine, N,O-bis(trimethylsilyl)-, trimethylsilyl ester	137174	007364-48-9	43
19	11.9249	0.4627	l-Alanine, N-(3-bromobenzoyl)-, tetradecyl ester	181794	1000314-08-6	27
20	12.7305	0.6058	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	152353	038166-11-9	83
21	13.8222	1.4111	1-Naphthalenemethanol	28421	004780-79-4	38
22	14.2664	0.5882	Per-O-(trimethylsilyl)-.beta.-l-idofuranuronic acid	187103	1000072-41-3	32
23	15.6367	0.3732	Xylonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone, D-	158612	010589-36-3	43
24	15.855	0.3914	Phosphoric acid, bis(trimethylsilyl) 2,3-bis[(trimethylsilyl)oxy]propyl ester	181044	031038-11-6	83
25	16.0734	0.5218	Glucofuranoside, methyl 2,3,5,6-tetrakis-O-(trimethylsilyl)-, .alpha.-D-	183112	006736-96-5	64
26	16.239	0.7534	Silane, (1,2,4,5-cyclohexanetetrayltetraoxy)tetrakis[trimethyl-	178056	100258-68-2	64

27	16.3218	0.4525	.alpha.-D-Galactofuranose, 1,2,3,5,6-pentakis-O-(trimethylsilyl)-	186561	055529-72-1	74
28	16.367	1.3673	D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186549	055529-69-6	59
29	16.4799	0.8067	D-Xylopyranose, 1,2,3,4-tetrakis-O-(trimethylsilyl)-	178316	055555-45-8	72
30	16.7058	0.4725	Phosphinic acid, diphenyl-, dimer	178106	1000164-07-2	43
31	16.8037	0.6427	1,3,5-Triazine, 2,4,6-tris[(trimethylsilyl)oxy]-	150013	060739-94-8	40
32	17.1575	1.4032	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186554	002775-90-8	91
33	17.2479	0.373	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	86
34	17.6092	1.0894	D-Mannopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186548	055529-69-6	53
35	17.7598	0.5003	L-Ascorbic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-	181475	055517-56-1	64
36	18.0083	1.605	Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-	186545	006736-99-8	87
37	18.0986	0.4554	Arabinose, 2,3,4,5-tetrakis-O-(trimethylsilyl)-	178314	001768-95-2	53
38	18.7612	1.7578	Hexadecanoic acid, trimethylsilyl ester	141306	055520-89-3	83
39	19.243	0.3705	Ferulic acid, trimethylsiloxy, trimethylsilyl ester	146526	067460-51-9	90
40	19.5969	0.3931	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170036	010586-03-5	87
41	20.5305	2.4716	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	92
42	20.5756	0.3658	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	47
43	20.9747	2.604	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186554	002775-90-8	83
44	21.1554	0.4007	Talose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186536	056192-85-9	64
45	22.5558	0.5604	Pyridine-2,5-dicarboxylic acid bis-cyclopropylamide	88468	1000294-44-0	45
46	22.616	7.8586	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	68
47	22.6988	0.6803	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	43
48	22.7741	0.3931	6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	70549	016489-90-0	59
49	22.872	0.6759	Mannonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181662	055515-30-5	35
50	23.1279	1.907	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	50
51	23.2635	0.3642	Benzene, 1,3-dichloro-5-(1,1-dimethylethyl)-2-methoxy-	79530	055191-16-7	32
52	23.4668	17.222	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	81
53	23.5571	9.7276	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	47
55	26.7494	1.1988	Melibiose, octakis(trimethylsilyl)-	190713	086087-85-6	58
56	27.2538	0.6975	2-Ethylacridine	62222	055751-83-2	38
57	27.5549	0.5567	1-Monolinoleoylglycerol trimethylsilyl ether	184354	054284-45-6	1
58	27.6152	0.5458	3-Bromo-5-ethoxy-4-hydroxybenzaldehyde	88284	003111-37-3	38
59	28.2702	1.3893	Benzo[h]quinoline, 2,4-dimethyl-	62243	000605-67-4	35

Table 8. Automated database search for sample 'WT16'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_21.D						
PBM Apex						
Mon Dec 10 16:38:52 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2304	28.9687	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39868	000920-68-3	94
2	4.4864	0.7521	Phenol, 4-(1-methyl-1-phenylethyl)-	66039	000599-64-4	10
3	5.3372	1.3907	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	72
4	5.5857	0.9135	N-(2-Chloroethyl)-N-ethylaniline	45198	000092-49-9	38
5	6.3686	0.6465	Hexestrol di-TMS	174302	070244-15-4	59
6	6.5945	0.9053	3-Fluorobenzoic acid, cyclopentyl ester	62598	1000279-04-5	41
7	6.73	2.0246	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71658	017887-80-8	91
8	6.7903	1.3595	Silane, [(1-methyl-1,3-propanediyl)bis(oxy)]bis[trimethyl-	80701	056771-47-2	64
9	7.4378	1.2818	l-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester	80612	027844-07-1	78
10	7.7766	0.905	Phenol, 4-t-butyl dimethylsilyloxy-	74118	108534-47-0	14
11	9.0038	3.9	Benzaldehyde, 3-(4-methoxyphenoxy)-	77177	062373-80-2	27
12	9.3049	2.0693	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118835	005630-82-0	90
13	9.704	1.6998	Trimethyl 2-methoxypropane-1,2,3-tricarboxylate	90104	1000110-15-7	37
14	9.9072	2.3275	Silanol, trimethyl-, phosphate (3:1)	133673	010497-05-9	93
15	10.743	0.75	3H-Indole, 2,3,3-trimethyl-	29173	001640-39-7	11
16	11.0742	0.999	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	180131	019127-15-2	53
17	11.925	0.8281	2-(4-Methoxyphenyl)benzoic acid	77166	1000305-27-1	35
18	13.2275	1.6319	2-Piperidinecarboxylic acid, 1-(trimethylsilyl)-, trimethylsilyl ester	107290	055255-44-2	59
19	13.4007	0.7923	Lycopodan-5-one, 12-hydroxy-15-methyl-, (15R)-	100647	006900-92-1	64
20	14.9064	3.9308	L-Asparagine, N,N2-bis(trimethylsilyl)-, trimethylsilyl ester	151403	055649-62-2	94
21	18.7612	3.6572	Hexadecanoic acid, trimethylsilyl ester	141309	055520-89-3	93
22	20.5305	5.2414	Octadecanoic acid, trimethylsilyl ester	155418	018748-91-9	92
23	20.9747	0.6479	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	59
24	22.616	4.5007	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	56
25	23.128	1.4156	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	38
26	23.4668	12.1143	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl	190724	019159-25-2	91

			2,3,4,6-tetrakis-O-(trimethylsilyl)-			
27	23.5572	6.0561	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	41
28	26.6214	4.5873	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-	188504	027864-29-5	46
29	27.2539	1.6711	1,1,1,3,5,5,5-Heptamethyltrisiloxane	73166	001873-88-7	42

Table 9. Automated database search for sample 'WT25'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z113012_22.D						
PBM Apex						
Mon Dec 10 16:40:17 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.1175	0.4537	Trisiloxane, octamethyl-	82775	000107-51-7	78
2	4.2455	15.9827	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	95
3	4.3584	0.3484	Ethanimidic acid, N-(trimethylsilyl)-, trimethylsilyl ester	59184	010416-59-8	47
4	5.3447	0.9292	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	90
5	5.5932	0.4945	Benzenesulfonamide, N-(3-chloropropyl)-N-methyl-	89598	074810-82-5	37
6	6.3762	0.3279	Tetrasiloxane, decamethyl-	130463	000141-62-8	45
7	6.6021	0.5087	N-(4-Nitro-1,8-naphthalimido)-4-fluorobenzamide	164772	300690-90-8	43
8	6.7301	1.0082	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71657	017887-80-8	86
9	6.7978	0.611	Ethanedioic acid, bis(trimethylsilyl) ester	81389	018294-04-7	52
10	7.4378	3.784	L-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester	80610	027844-07-1	80
11	7.7465	0.6522	.beta.-Amino isobutyric acid, bis(trimethylsilyl)-	89616	058521-52-1	53
12	9.0038	2.2012	1,4-Dimethylphenoxathin	77224	016314-44-6	27
13	9.0866	0.4398	N,O-Bis-(trimethylsilyl)valine	99066	015984-93-7	45
14	9.3049	1.3185	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118833	005630-82-0	86
15	9.704	0.6592	Acetamide, N-(7,8-dihydro-1-ethenyl-6H-cyclohepta[b]pyrrol-7-yl)-N-methyl-	78658	313996-62-2	45
16	9.8997	3.244	Silanol, trimethyl-, phosphate (3:1)	133673	010497-05-9	94
17	10.5246	0.4165	Butanedioic acid, bis(trimethylsilyl) ester	99521	040309-57-7	76
18	10.6677	0.332	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137602	038191-87-6	72
19	10.743	0.3763	5-Methyl-thieno[2,3-d]thiazol-2-ylamine	36624	041940-59-4	11
20	11.0667	0.6984	L-Serine, N,O-bis(trimethylsilyl)-, trimethylsilyl ester	137174	007364-48-9	52
21	11.398	0.356	N,O,O-Tris(trimethylsilyl)-L-threonine	145070	007537-02-2	43
22	11.9325	0.4054	Bis[p-cyanophenyl]acetylene	77444	005216-36-4	27
23	12.7306	1.5379	Malic acid, O-(trimethylsilyl)-, bis(trimethylsilyl)ester	152351	107241-82-7	91
24	13.235	0.38	Cyclopentanecarboxylic acid, 1-amino-, bis(trimethylsilyl) deriv.	107287	056273-05-3	64
25	13.4007	0.3323	1-Allyl-2-imino-10-oxo-1,10-dihydro-2H-1,9,10a-triazaanthracene-3-carboxylic acid, methyl ester	130761	1000311-49-4	59

26	14.3267	1.6836	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	180131	019127-15-2	83
27	14.8989	1.1026	Asparagine, O,O',N-tris(trimethylsilyl)-	151401	1000141-39-1	90
28	15.0721	0.8387	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	180129	019127-15-2	83
29	15.7647	2.1045	1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)-	168234	055530-71-7	91
30	16.3595	2.0556	1-Cyclohexene-1-carboxylic acid, 3,4,5-tris[(trimethylsilyl)oxy]-, trimethylsilyl ester, [3R-(3.alpha.,4.alpha.,5.beta.)]-	181279	055520-78-0	80
31	16.4875	0.9737	.alpha.-D-Glucopyranoside, methyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	183103	002641-79-4	64
32	16.8037	1.5395	1,3,5-Triazine, 2,4,6-tris[(trimethylsilyl)oxy]-	150013	060739-94-8	59
33	16.9995	0.3401	Gulonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181659	055528-75-1	47
34	17.1576	1.6578	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	91
35	17.6093	1.3773	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	64
36	17.7524	0.4317	L-Ascorbic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-	181475	055517-56-1	72
37	18.0084	2.1865	l-Fucose, tetra-TMS-ether	180126	117307-13-8	80
38	18.7613	1.5173	Hexadecanoic acid, trimethylsilyl ester	141311	055520-89-3	97
39	19.0473	0.325	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, scyllo-	188713	014251-18-4	64
40	19.597	0.3202	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170034	010586-03-5	76
41	20.523	2.1118	Octadecanoic acid, trimethylsilyl ester	155420	018748-91-9	96
42	20.9748	2.8128	Glycoside, .alpha.-methyl-trtrakis-O-(trimethylsilyl)-	183098	1000156-15-2	72
43	22.5483	0.3437	Per-O-trimethylsilyl-(3-O-.beta.-d-mannopyranosyl-d-glucitol)	190759	1000072-62-9	45
44	22.6161	2.0219	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	64
45	22.7741	0.3648	2-Isobenzazole, 1,3-dioxo-2-ethyl-5,6-methylenedioxy-	70356	003990-41-8	64
46	23.128	0.9097	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	45
47	23.4668	16.1563	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	91
48	23.5572	7.9098	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	49
49	24.95	0.5613	1H-Indole, 3-phenyl-2-(heptafluoropropyl)-	157468	168104-45-8	37
50	25.1232	0.3709	3,3,5,5,7,7,9,9,11,11,13,13-Dodecamethyl-1,15-bis(1,3,3,5,5-pentamethyl-2,4,6-trioxa-1,3,5-trisilacyclohexyl)-4,6,8,10,12-tetraoxa-3,5,7,9,11-tetrasilapentadecane	190687	118229-41-7	42
51	25.8987	0.622	Indole-3-carboxaldehyde, 4-tolylhydrazone	91351	1000262-65-3	20
52	26.1019	0.3521	2-Ethylacridine	62222	055751-83-2	38
53	26.6214	1.6935	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-	188504	027864-29-5	37
54	26.7494	0.7254	Maltose, octakis(trimethylsilyl)-	190709	033428-94-3	64
55	26.7946	0.916	1,3,5-Triazine, 2,4,6-tris[(trimethylsilyl)oxy]-	150013	060739-94-8	30

56	27.2539	1.0032	3-Methylindole-2-carboxylic acid, 4,5,6,7-tetrahydro-, ethyl ester	62156	037945-37-2	53
57	27.3291	3.3347	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[3-chloro-2-[(trimethylsilyl)oxy]propyl]-1,3-dimethyl-5-(2-propenyl)-	156873	055836-74-3	27

Table 10. Automated database search for sample 'T18-3'

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z121012_05.D						
PBM Apex						
Tue Dec 11 00:14:19 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2003	3.5154	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	95
2	4.3283	0.0864	3-Methyl-1-dimethyl(chloromethyl)silyloxybutane	53229	018279-90-8	43
3	5.2243	0.0787	Guanosine	113620	000118-00-3	32
4	5.3221	0.3241	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47703	001000-70-0	70
5	5.5781	0.145	Isophthalaldehyde	14759	000626-19-7	38
6	6.5945	0.1228	Benzoyl chloride, 2-fluoro-	28677	000393-52-2	27
7	6.7225	0.2651	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71656	017887-80-8	72
8	6.7903	0.2375	Silane, [(1-methyl-1,3-propanediyl)bis(oxy)]bis[trimethyl-	80701	056771-47-2	72
9	7.2872	0.2619	N-Trimethylsilyl-n-heptylamine	47984	017940-17-9	27
10	7.4378	0.5571	l-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester	80612	027844-07-1	80
11	7.7766	0.1241	Benzenamine, N-phenyl-	35735	000122-39-4	27
12	8.9962	0.3436	1,4-Dimethylphenoxathin	77224	016314-44-6	35
13	9.2974	0.3634	Propanoic acid, 3-[bis(trimethylsilyl)amino]-2-methyl-, trimethylsilyl ester	136129	055125-15-0	86
14	9.704	0.1912	4,6-Dioxoheptanoic acid bis(trimethylsilyl) ester	125672	101329-13-9	28
15	9.8997	0.2648	Silanol, trimethyl-, phosphate (3:1)	133674	010497-05-9	91
16	10.3891	0.1114	2-Pentenoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	98294	055045-17-5	86
17	10.6601	0.2325	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137600	038191-87-6	86
18	10.743	0.3154	5,6-Dihydro-2-mercapto-4-methylthieno(2,3-d)pyrimidine	46364	005909-38-6	30
19	11.0667	0.0827	Galacturonic acid, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester	187112	056192-87-1	59
20	11.925	0.1357	Triphenylene	77461	000217-59-4	27
21	12.5123	0.1287	Pyruvic acid oxime, bis(trimethylsilyl)- deriv.	90067	051621-44-4	41
22	12.7306	0.2453	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	152352	038166-11-9	87

23	13.1221	0.0908	1H-Indole-3-acetic acid, 5-methoxy-1-(trimethylsilyl)-, trimethylsilyl ester	152141	055887-55-3	47
24	13.4007	0.1704	Trimethyl(2,6 ditert.-butylphenoxy)silane	110721	010416-73-6	64
25	13.6265	0.1009	Benzothiazole, 6-methoxy-2-(4-nitrobenzylidenamino)-	132565	016779-15-0	50
26	13.9352	0.2107	2,6-Bis[4-cyanostyryl]pyridine	144319	061973-88-4	27
27	14.0482	0.1352	2-Butenoic acid, 2-[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester	142200	1000221-69-9	32
28	14.3117	0.2091	N,o,o'-Tris-(trimethylsilyl)-6-hydroxy-2-aminohexanoic acid	158301	066434-54-6	89
29	15.3808	0.093	Propanedioic acid, (trimethylsilyl)-, bis(trimethylsilyl) ester	136518	056051-48-0	32
30	15.7647	1.194	1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)-	168235	055530-71-7	99
31	16.239	1.0338	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	64
32	16.3219	1.3985	.alpha.-DL-Lyxofuranoside, methyl 2,3,5-tris-O-(trimethylsilyl)-	164977	056390-03-5	72
33	16.367	2.4484	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	186550	030645-02-4	90
34	16.4574	0.1377	1-Pentamethyldisilyloxydecane	117065	1000216-85-1	40
35	16.4875	0.1098	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	78
36	16.6607	0.0899	Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	178320	055399-49-0	72
37	16.7134	0.1223	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	186550	030645-02-4	64
38	16.8037	0.4099	Pyrrole, 2-(2-naphthyl)-3,5-diphenyl-	150362	170238-88-7	38
39	17.1576	2.2386	.alpha.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186556	003327-61-5	91
40	17.2479	0.1131	Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, .beta.-d-	186562	001769-00-2	80
41	17.3232	0.606	1-Diphenyl(tert-butyl)silyloxy-4-methoxybenzene	158155	1000307-86-6	39
42	17.6018	0.145	D-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186546	006736-94-3	72
43	17.7524	0.2106	L-Ascorbic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-	181475	055517-56-1	72
44	17.79	0.2442	Naphtho[2,3-c]furan-1(3H)-one, 4-(3,4-dimethoxyphenyl)-3a,4,9,9a-tetrahydro-6,7-dimethoxy-, [3aS-(3a.alpha.,4.alpha.,9a.beta.)]-	166401	025925-39-7	27
45	18.0084	3.4293	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186540	006736-97-6	91
46	18.445	0.1576	Bis(tricarbonyliron)(Fe-Fe), (.mu.-bromo)[.mu.-.eta.-1:.eta.-2-2-(phenanthryl)vinyl]	187380	1000153-98-6	1
47	18.7613	0.7468	Hexadecanoic acid, trimethylsilyl ester	141306	055520-89-3	93
48	19.0473	0.6741	Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, muco-	188711	029412-26-8	93
49	19.597	0.1269	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170035	010586-03-5	90
50	20.5305	1.1886	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	94
51	20.9748	1.684	Talose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186536	056192-85-9	86
52	21.8556	0.153	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	35
53	22.1944	0.2025	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	53
54	22.33	0.0791	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	35
55	22.4052	0.209	11H-Benzo[a]carbazole	69222	000239-01-0	38

56	22.4579	0.1023	.alpha.-L-Galactopyranose, 6-deoxy-1,2,3,4-tetrakis-O-(trimethylsilyl)-	180138	032727-30-3	58
57	22.5558	0.8037	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	46
58	22.6161	0.1734	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	64
59	22.6989	0.7846	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	35
60	22.7741	0.1644	4-(1-Methyl-3-oxobutylideneamino)benzoic acid	70407	088074-23-1	43
61	22.857	0.1968	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	37
62	23.128	0.2139	Guaicol-.beta.-d-glucopyranoside, pentakis(O-trimethylsilyl)-	187749	1000108-99-2	27
63	23.3388	0.1214	2-Dimethyl(pentafluorophenyl)silyloxyadamantane	163676	1000283-08-0	46
64	23.4969	65.0127	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	74
65	23.5647	0.7613	[4-Bromo-2-(hydrazono-phenyl-methyl)-phenyl]-carbamic acid, ethyl ester	157451	1000318-37-6	87
66	23.7981	0.1609	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	53
67	26.757	1.364	.alpha.-l-Mannopyranoside, methyl 6-deoxy-2,3,4-tris-O-(trimethylsilyl)-	169447	056271-60-4	72
68	26.9	0.1479	Pyrimidin-2(1H)-thione, 5-[5-(4-morpholyl)-2-furfurylidene]-4,6(3H,5H)-dioxo-	128833	339274-16-7	47
69	27.2539	0.3122	Tetrasiloxane, decamethyl-	130465	000141-62-8	27
70	27.3291	0.2346	2-Morpholino-2-phenyl-1,3-indandione	129087	006549-42-4	56
71	28.2853	1.1503	Per-O-trimethylsilyl-(3-O-.alpha.-d-mannopyranosyl-4-O-.beta.-d-glucopyranosyl-d-glucitol)	190822	1000072-62-8	37

Table 11. Automated database search for sample 'T51-1'

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PBM Apex						
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PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.223	5.2694	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	94
2	4.3434	0.1166	2,2-Dimethyl-1-pentamethyldisilanyloxypropane	69409	1000216-94-2	59
3	5.2319	0.1074	Phenol, 2,6-dimethyl-4-nitroso-	23860	013331-93-6	37
4	5.3297	0.4847	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	47
5	5.5857	0.2075	4-Methyl-benzofurazan	14689	029091-40-5	25
6	6.3687	0.1171	Tetrasiloxane, decamethyl-	130463	000141-62-8	72
7	6.5946	0.1888	4-Fluorobenzoic acid, 3,5-difluorophenyl ester	93138	1000299-04-8	38
8	6.7226	0.3809	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	59
9	6.7904	0.311	Silane, trimethyl[1-methyl-2-oxo-2-(trimethylsilyl)ethoxy]-, (R)-	70223	055255-93-1	78
10	7.2873	0.2745	L-Proline, 1-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester	149160	107715-91-3	22
11	7.4378	0.9456	l-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester	80612	027844-07-1	93
12	7.7766	0.1579	1,3-Cyclopentadiene, 1,2,3,4-tetrachloro-	58584	000695-77-2	32
13	8.9963	0.1797	Carbonic acid, 3-methylphenyl phenyl ester	77197	017146-02-0	46
14	9.2975	0.4622	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118835	005630-82-0	74
15	9.8923	2.2178	Silanol, trimethyl-, phosphate (3:1)	133671	010497-05-9	97
16	10.6677	0.4694	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137600	038191-87-6	80
17	10.743	0.2971	1,4-Benzenediamine, N-phenyl-	45916	000101-54-2	18
18	10.9011	0.1381	Butanedioic acid, bis(trimethylsilyl) ester	99522	040309-57-7	72
19	11.0668	0.1846	.beta.-l-Galactopyranoside, methyl 6-deoxy-2,3,4-tris-O-(trimethylsilyl)-	169448	056271-59-1	50
20	11.9251	0.1892	Triphenylene	77462	000217-59-4	22
21	12.5123	0.2109	N,N,o'-Tris-(trimethylsilyl)aspartic acid	152004	015985-05-4	49
22	12.7307	0.7743	Malic acid, tris(trimethylsilyl) ester	152350	065143-63-7	91
23	12.9942	0.1164	1,4-Diboracyclohexane, 1,4-diethyl-2,5-bis(trimethylsilyl)-	111648	1000160-14-7	37
24	13.1222	0.1517	L-Aspartic acid, N-(trimethylsilyl)-, bis(trimethylsilyl) ester	152006	055268-53-6	64
25	13.4007	0.3755	Trimethyl(2,6 ditert.-butylphenoxy)silane	110721	010416-73-6	78
26	13.8224	0.2971	Silane, (2,2-dimethylpropoxy)trimethyl-	29978	018246-63-4	35

27	13.9428	0.114	2H-1-Benzopyran-2-one, 3-(1,1-dimethyl-2-propenyl)-6-methoxy-7-[(trimethylsilyl)oxy]-	143541	055682-68-3	38
28	14.0482	0.1308	2-Butenoic acid, 2-[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester	142200	1000221-69-9	50
29	14.1762	0.1526	2-Pentenedioic acid, 2-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	157726	055590-97-1	38
30	14.2666	0.1212	3-Bromo-5-ethoxy-4-hydroxybenzaldehyde	88284	003111-37-3	50
31	14.3117	0.2254	N,o,o'-Tris-(trimethylsilyl)-6-hydroxy-2-aminohexanoic acid	158301	066434-54-6	81
32	15.2754	0.1866	2-Propenoic acid, 2-[(trimethylsilyl)oxy]-3-[4-[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester	170038	027750-74-9	32
33	15.3808	0.1061	2-Pentenedioic acid, bis(trimethylsilyl) ester	107740	055255-43-1	37
34	15.6368	0.1495	2-Ketobutyric acid oxime, bis(trimethylsilyl)-	99019	1000078-99-8	35
35	15.7648	1.4967	1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)-	168234	055530-71-7	68
36	16.0735	0.144	Hexanedioic acid, 2-trimethylsilyloxy-, bis(trimethylsilyl) ester	164311	1000292-69-7	35
37	16.2316	0.2999	Pseudo uridine penta-tms	188529	053294-25-0	59
38	16.322	0.4155	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	83
39	16.3671	0.6428	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	186553	030645-02-4	91
40	16.48	0.4263	Talose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186536	056192-85-9	58
41	16.8038	0.3202	7-Methoxy-.alpha.-tetraloxime, toluenesulfonate(ester)	150169	099833-87-1	35
42	17.1577	0.7929	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186555	002775-90-8	90
43	17.248	0.2025	Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-, D-	186551	019126-99-9	87
44	17.3233	0.1772	Ethene, 1-(anthracen-9-yl)-2-(4-cyanophenyl)-, (E)	127980	1000163-13-9	9
45	17.5793	0.1598	Cinnamic acid, 3,4-bis(trimethylsiloxy)-, methyl ester	146527	022020-29-7	17
46	17.7826	0.1153	Acetic acid, [o-(trimethylsiloxy)phenyl]-, trimethylsilyl ester	121891	027750-52-3	25
47	18.0084	1.1848	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186538	006736-97-6	90
48	18.7613	0.7594	Hexadecanoic acid, trimethylsilyl ester	141306	055520-89-3	86
49	19.0474	0.6117	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	188707	002582-79-8	94
50	19.2432	0.1511	Trimethylsilyl 3-methoxy-4-(trimethylsilyloxy)cinnamate	146531	010517-09-6	94
51	19.597	0.2583	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170036	010586-03-5	91
52	20.5231	1.0824	Octadecanoic acid, trimethylsilyl ester	155418	018748-91-9	89
53	20.9748	3.2873	Talose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186536	056192-85-9	80
54	21.8557	0.1895	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	35
55	22.1945	0.1539	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	42
56	22.5483	0.5557	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	38
57	22.6161	1.2538	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl	190724	019159-25-2	58

			2,3,4,6-tetrakis-O-(trimethylsilyl)-			
58	22.6989	0.5168	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	43
59	22.7742	0.1626	2-Isobenzazole, 1,3-dioxo-2-ethyl-5,6-methylenedioxy-	70356	003990-41-8	45
60	22.8646	0.2047	1H-Indole-3-carboxaldehyde, 1-(trimethylsilyl)-	69080	074367-39-8	14
61	23.1281	0.9923	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	43
62	23.3841	0.1908	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	38
63	23.4819	59.3009	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	50
64	23.5648	2.1286	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	53
65	23.9487	0.1414	Thiazolo[3,2-b]1,2,4-triazole, 2-trifluoromethyl-6-methyl-5-(2-phenyl-4-pyrimidyl)-	157435	266679-25-8	38
66	25.6277	0.1238	(3-Hydroxy-4-methoxyphenyl)ethylene glycol tris(trimethylsilyl) ether	171195	1000072-20-5	50
67	25.9063	0.1311	Benzo[a]4,7-phenantrolin-9(7H)-one, 8,10,11,12-tetrahydro-8-(3-methyl-2-thienyl)-	150798	1000271-48-8	45
68	26.6215	1.2375	Diethyl[3-[n-octadecylmercapto]-p-n-butylanilinomethylene]malonate	188524	1000214-74-7	7
69	26.7495	1.8898	.alpha.-D-Glucopyranoside, methyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	183103	002641-79-4	78
70	27.2539	0.3313	Benzo[h]quinoline, 2,4-dimethyl-	62243	000605-67-4	38
71	27.3292	0.3078	Cyano(4,4,6-trimethyl-2-oxo-4H-pyrrolo[3,2,1-ij]quinolin-1-ylidene)acetic acid, ethyl ester	137945	1000316-68-1	38
72	27.5476	0.1244	1-Monolinoleoylglycerol trimethylsilyl ether	184354	054284-45-6	4
73	28.2854	1.7233	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	68

Table 12. Automated database search for sample 'T51-2'

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PBM Apex						
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PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.2303	4.6636	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	95
2	4.3433	0.1092	1-Pentamethyldisilyloxydodecane	134511	1000216-85-3	59
3	4.4863	0.1004	Pyrimidine, 2-fluoro-5-chloro-4-amino-	21460	000155-10-2	38
4	5.2392	0.1422	Phenol, 2,6-dimethyl-4-nitroso-	23860	013331-93-6	43
5	5.3371	0.4245	Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	42
6	5.5855	0.1938	Iron, (.eta.6-benzene)[(1,2,3,4-.eta.)-1,3-cyclohexadiene]-	66975	071265-76-4	16
7	6.3686	0.1015	Tetrasiloxane, decamethyl-	130463	000141-62-8	78
8	6.5944	0.1514	2-Fluorobenzoic acid, 6-ethyl-2-octyl ester	111916	1000278-96-7	35
9	6.7299	0.3369	1,3-Dimethyl-5-dimethyl(trimethylsilylmethyl)-silyloxycyclohexane	106634	1000216-95-6	59
10	6.7902	0.3017	Butane, 2,3-bis(trimethylsiloxy)-	80688	053274-85-4	59
11	7.2871	0.3101	Propane(dithioic) acid, ethyl ester	14558	000998-79-8	22
12	7.4377	0.8169	l-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester	80612	027844-07-1	86
13	7.7765	0.1325	1,1'-Biphenyl, 4-azido-	53566	031656-91-4	38
14	9.2973	0.4168	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118833	005630-82-0	90
15	9.8921	1.6202	Silanol, trimethyl-, phosphate (3:1)	133673	010497-05-9	94
16	10.66	0.415	Propanoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	137600	038191-87-6	96
17	10.7429	0.2201	2,7-Diamino-quinoline-3-carbonitrile	45697	1000187-24-4	15
18	10.901	0.096	2-Hexenoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	107812	069796-61-8	59
19	10.9988	0.1103	2-Butenedioic acid (E)-, bis(trimethylsilyl) ester	98245	017962-03-7	64
20	11.9249	0.1257	1H-Indole, 3-(2,5-dimethylthiazol-4-yl)-	77057	1000304-18-5	35
21	12.5122	0.3142	7H-Furo(3,2-g)(1)benzopyran-7-one, 9-(2,3-dihydroxy-3-methylbutoxy)-4-methoxy-, (R)-	144599	000482-25-7	47
22	12.7305	1.5372	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	152353	038166-11-9	91
23	13.122	0.2008	N,N,o'-Tris-(trimethylsilyl)aspartic acid	152004	015985-05-4	91
24	13.4006	0.1681	Trimethyl(2,6 ditert.-butylphenoxy)silane	110721	010416-73-6	72
25	13.8222	0.0954	3,8-Dioxa-2,9-disiladec-5-ene, 2,2,9,9-tetramethyl-, (E)-	79474	053326-59-3	43

26	14.0556	0.0975	1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-6-methoxy-1,4a-dimethyl-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-	107004	016826-83-8	43
27	14.1685	0.1077	2-Pentenedioic acid, 2-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	157728	055590-97-1	38
28	14.3116	0.2338	Buta-1,3-diyne, 1,4-bis(2-methoxycarbonylcyclopropyl)-	89165	1000268-72-3	92
29	15.7646	2.0579	1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (Z)-	168235	055530-71-7	91
30	16.2314	0.3067	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-	186543	019126-98-8	83
31	16.3218	0.4096	Pseudo uridine penta-tms	188529	053294-25-0	59
32	16.3669	0.6161	.alpha.-DL-Lyxopyranose, 1,2,3,4-tetrakis-O-(trimethylsilyl)-	178327	056271-67-1	59
33	16.4799	0.4027	.alpha.-D-Galactopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186560	032166-80-6	72
34	16.8036	0.3364	Glutaconic acid, tris(trimethylsilyl)-(ester)	150440	1000079-68-7	38
35	17.1575	0.7182	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	180129	019127-15-2	91
36	17.2478	0.1481	D-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	186546	006736-94-3	76
37	17.3231	0.2213	O,O,O'-Tris-trimethylsilylmalonate	136517	040333-06-0	56
38	17.7523	0.1714	L-Ascorbic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-	181475	055517-56-1	27
39	18.0083	1.0584	.beta.-D-Glucopyranose, 1,2,3,4,6-pentakis-O-(trimethylsilyl)-	186555	002775-90-8	91
40	18.4449	0.1221	Propanedioic acid, (trimethylsilyl)[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	172943	055530-65-9	38
41	18.7612	0.5673	Hexadecanoic acid, trimethylsilyl ester	141307	055520-89-3	89
42	19.0472	0.6228	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	188704	002582-79-8	91
43	19.5969	0.1976	Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate	170034	010586-03-5	90
44	19.6345	0.1527	1,1,2,2-Tetra(trimethylsilyl)3,4-bis(trimethylsiloxy)3,4-diphenyl-1,2-silacyclobutane	189991	060154-99-6	38
45	20.5229	0.8171	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	99
46	20.9747	2.7341	2-O-Glycerol-.alpha.-d-galactopyranoside, hexa-TMS	189811	1000098-09-0	86
47	21.8555	0.1749	Xanthine, 1,3-diethyl-8-[4-[[[ethylamino]carbonyl]methoxy]phenyl]-	166731	104576-48-9	27
48	22.1943	0.2266	D-Arabinonic acid, 2,3,5-tris-O-(trimethylsilyl)-, .gamma.-lactone	158615	032384-55-7	43
49	22.3223	0.1022	Hydroquinone-.beta.-d-glucopyranoside,pentakis(trimethylsilyl)-	189079	1000108-97-3	37
50	22.4051	0.123	Allonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone	181656	055515-34-9	32
51	22.5482	0.6524	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	38
52	22.616	0.9165	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190724	019159-25-2	52
53	22.6988	0.5064	Thymol-.beta.-d-glucopyranoside, tetrakis(O-trimethylsilyl)-	188461	1000108-99-1	38
54	22.774	0.145	1H-Isoindole-5-carboxylic acid, 2-ethyl-1,3-dioxo-2,3-dihydro-	70360	1000304-22-8	50
55	22.8644	0.1972	Per-O-(trimethylsilyl)-.alpha.-D-galactofuranuronic acid	187108	064665-61-8	27
56	23.1279	0.8789	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	42
57	23.3839	0.1237	D-Turanose, heptakis(trimethylsilyl)-	190607	060065-05-6	46

58	23.4893	62.9409	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	55
59	23.5646	2.2727	[4-Bromo-2-(hydrazono-phenyl-methyl)-phenyl]-carbamic acid, ethyl ester	157451	1000318-37-6	74
60	23.9486	0.1954	Scopolin, tetra(trimethylsilyl)-	189268	1000108-98-9	38
61	25.8835	0.1211	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	187862	019095-24-0	38
62	26.6213	1.0047	[2,2'-Binaphthalene]-8,8'-dicarboxaldehyde, 1,1',6,6',7,7'-hexamethoxy-3,3'-dimethyl-5,5'-bis(1-methylethyl)-	188504	027864-29-5	9
63	26.7493	1.7106	Melibiose, octakis(trimethylsilyl)-	190713	086087-85-6	86
64	27.2538	0.3317	Silane, 1,4-phenylenebis(trimethyl-	72522	013183-70-5	45
65	27.329	0.248	(1H-Benzoimidazol-2-yl)-[4-(4-methyl-piperazin-1-yl)-phenyl]-amine	129071	056642-89-8	38
66	27.5474	0.1149	1H-Pyrrole-2,5-dione, 1-(4-chlorophenyl)-	61904	001631-29-4	35
67	28.2777	1.809	.alpha.-D-Glucopyranoside, 1,3,4,6-tetrakis-O-(trimethylsilyl)-.beta.-D-fructofuranosyl 2,3,4,6-tetrakis-O-(trimethylsilyl)-	190723	019159-25-2	64

Table 13. Automated database search for MSTFA blank (10:1 split injection)

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z121012_03.D						
PBM Apex						
Tue Dec 11 00:22:18 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	5.0811	23.0854	Acetamide, 2,2,2-trifluoro-N,N-bis(trimethylsilyl)-	96933	021149-38-2	86
2	5.4877	1.228	Pantoyl lactone, trimethylsilyl	58782	042411-50-7	38
3	5.7286	0.6393	1,3-Dichloro-2-propanol, trimethylsilyl ether	57395	007453-13-6	37
4	5.8114	1.4181	Butyrolactone	1620	000096-48-0	87
5	5.9394	4.7901	Silanameine, N,N'-methanetetraylbis[1,1,1-trimethyl-	47702	001000-70-0	68
6	6.0373	1.7108	Silanol, trimethyl-, propanoate	21056	016844-98-7	38
7	6.2029	3.4279	Iron, (.eta.6-benzene)[(1,2,3,4-.eta.)-1,3-cyclohexadiene]-	66975	071265-76-4	18
8	6.3836	0.6539	9-Chloropyrazino[2,3-c][2,7]naphthyridine	68131	1000147-79-9	12
9	6.4815	1.0313	Tetrasiloxane, decamethyl-	130465	000141-62-8	59
10	6.6923	1.6537	Methyltris(trimethylsiloxy)silane	130466	017928-28-8	68
11	6.9407	3.2309	3-Fluorobenzoic acid, 2-methylphenyl ester	78595	1000299-05-6	35
12	7.0311	5.87	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71657	017887-80-8	91
13	7.0838	3.0277	Silane, [(1-methyl-1,3-propanediyl)bis(oxy)]bis[trimethyl-	80702	056771-47-2	53
14	7.1515	1.3536	Sulfurous acid, bis(2-pentyl) ester	72264	1000309-15-3	25
15	7.6485	1.5072	Disiloxane, 1,3-bis(1,1-dimethylethyl)-1,1,3,3-tetramethyl-	88963	067875-55-2	59
16	7.9345	2.4449	Silane, bromotriethyl-	53057	001112-48-7	37
17	8.6197	2.4687	2-Pyrrolidinone	1516	000616-45-5	78
18	9.0187	10.9955	Carbonic acid, 3-methylphenyl phenyl ester	77197	017146-02-0	38
19	9.3199	5.9803	Cadaverine tri-TMS	135437	1000141-25-1	72
20	9.6813	3.2252	Quinoline, 4,8-dimethyl-	27978	013362-80-6	40
21	10.6675	0.8977	3-Chlorobicyclo(2.2.1)heptan-2-one oxime	29242	010499-35-1	25
22	10.7278	1.2205	Quinoline, 6-methoxy-	29084	005263-87-6	18
23	11.8195	1.0423	2,8-Dimethylphenoxathiin	77225	021797-73-9	14
24	11.8872	3.2515	1-Methylcyclooctanol	19259	059123-41-0	18
25	13.5963	0.6921	Hexadecanoic acid, tert-butyldimethylsilyl ester	161430	058160-87-5	32
26	15.2526	1.0108	4-Methyl-2,3-hexadien-1-ol	6379	1000196-09-6	50

27	18.7611	2.4984	Hexadecanoic acid, trimethylsilyl ester	141309	055520-89-3	96
28	20.5304	7.3933	Octadecanoic acid, trimethylsilyl ester	155417	018748-91-9	98
29	22.631	0.752	Heptadecane, 2,6,10,15-tetramethyl-	122447	054833-48-6	90
30	23.3914	0.7494	Hexacosane	159835	000630-01-3	93
31	24.1217	0.7496	Decane, 1-iodo-	103528	002050-77-3	81

Table 14. Automated database search for MSTFA blank (splitless injection)

C:\Users\ssmith\Desktop\Sample Analysis\12039 Traub\z121012_04.D						
PBM Apex						
Tue Dec 11 00:23:26 2012						
PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	4.223	63.7715	Silanamine, N,1,1,1-tetramethyl-N-(trimethylsilyl)-	39869	000920-68-3	96
2	4.3359	1.4537	3,4-Dimethyl-1-pentamethyldisilyloxycyclohexane	97178	1000245-74-0	45
3	4.9683	1.49	1,3-Dichloro-2-propanol, trimethylsilyl ether	57395	007453-13-6	38
4	5.3297	1.8688	1,5-Dihydro-4H-furo[3,4-d][1,3]thiazine-2,7-dione	37217	1000186-12-0	50
5	5.5857	1.9906	3-(Benzenesulfonyl-methyl-amino)-propionic acid	87094	1000297-41-1	22
6	6.3687	1.3898	Methyltris(trimethylsiloxy)silane	130466	017928-28-8	56
7	6.5946	1.5857	Methyl 3,3,3-trifluoro-2-(2-fluorobenzamido)lactate	121238	328391-88-4	25
8	6.7301	4.0979	3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-	71658	017887-80-8	78
9	7.7766	1.5967	Butyric acid, 3-bromo-, trimethylsilyl ester	84123	018301-67-2	16
10	8.9963	7.0178	1-Phenyl-3,9-dihydro-purine-2,6-dione	76905	1000317-91-3	22
11	9.2974	3.7937	Glycine, N,N-bis(trimethylsilyl)-, trimethylsilyl ester	118834	005630-82-0	90
12	9.704	1.2779	2H-Thiazolo[2,3-c][1,2,4]triazol-3-one, 6-methyl-5,6-dihydro-	28039	1000309-93-6	43
13	10.743	1.4413	Lauryl gallate	146690	001166-52-5	18
14	11.91	2.8832	dl-3-Acetamido-perhydro-3-methyl-2-oxofuran	28121	089910-27-0	35
15	18.7613	1.272	Hexadecanoic acid, trimethylsilyl ester	141306	055520-89-3	86
16	20.5306	3.0695	Octadecanoic acid, trimethylsilyl ester	155420	018748-91-9	86